SIMULATION OF OIL SLICK TRANSPORT IN GREAT LAKES CONNECTING CHANNELS

Volume I: Theory and Model Formulation

H.T. Shen
P.D. Yapa
M.E. Petroski

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION	1b. RESTRICTIVE MARKINGS
Unclassified	

2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION / AVAILABILITY OF REPORT
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE	Approved for public release; distribution unlimited

4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S)
Report No. 86-1	

6a. NAME OF PERFORMING ORGANIZATION	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION
Clarkson University		

6c. ADDRESS (City, State, and ZIP Code)	7b. ADDRESS (City, State, and ZIP Code)
Department of Civil and Environmental Engineering Potsdam, NY 13676	

8a. NAME OF FUNDING / SPONSORING ORGANIZATION U.S. Army Corps of Engineers	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
		DACA 33-85-C-0001

8c. ADDRESS (City, State, and ZIP Code)	10. SOURCE OF FUNDING NUMBERS			
Detroit District P.O. Box 1027 Detroit, MI 48231	PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.

11. TITLE (Include Security Classification)
Simulation of Oil Slick Transport in Great Lakes Connecting Channels; Volume I: Theory and Model Formulation

12. PERSONAL AUTHOR(S)
Shen, H.T., P.D. Yapa, M.E. Petroski

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM _____ TO _____	March 1986	80

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	oil slicks, analytical framework, river current simulation, lake circulation, advection, mechanical spreading, evaporation, dissolution, shoreline conditions

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

In this study, two computer models named as ROSS and LROSS are developed for simulating oil slick transport in rivers and lakes, respectively. The oil slick transformation processes considered in these models include advection, spreading, evaporation and dissolution. These models can be used for slicks of any shape originated from instantaneous or continuous spills in rivers and lakes with or without ice covers. Although developed for the need of the connecting channels in the upper Great Lakes, including the Detroit River, Lake St. Clair, St. Clair River, and St. Marys River, these models are site independent and can be used to other rivers and lakes. The programs are written in FORTRAN programming language to be compatible with FORTRAN77 compiler. The models are designed to be used on both mainframe and microcomputers.

20. DISTRIBUTION / AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE (Include Area Code)	22c. OFFICE SYMBOL
Jimmie L. Glover	(313) 226-7590	CENCE-PD-EA

DD Form 1473, JUN 86   *Previous editions are obsolete.*   SECURITY CLASSIFICATION OF THIS PAGE

SIMULATION OF OIL SLICK TRANSPORT
IN GREAT LAKES CONNECTING CHANNELS

Volume I: Theory and Model Formulation

by

Hung Tao Shen, Poojitha D. Yapa and Mark E. Petroski

Report No. 86-1

Department of Civil and Environmental Engineering
Clarkson University
Potsdam, New York 13676

March 1986

PREFACE

The growing concern over the possible impacts of oil spills on aquatic environments has led to the development of a large number of computer models for simulating the transport and spreading of oil slicks in surface water bodies. Almost all of these models were developed for coastal environments. With the increase in inland navigation activities, oil slick simulation models for rivers and lakes are needed.

In this study, two computer models named as ROSS and LROSS are developed for simulating oil slick transport in rivers and lakes, respectively. The study was orignated by the · Detroit District, U.S. Army Corps of Engineers in relation to the Great Lakes limited navigation season extension study. The oil slick transformation processes considered in these models include advection, spreading, evaporation and dissolution. These models can be used for slicks of any shape originated from instantaneous or continuous spills in rivers and lakes with or without ice covers. Although developed for the need of the connecting channels in the upper Great Lakes, including the Detroit River, Lake St. Clair, St. Clair River, and St. Mary's River, these models are site independent and can be used to other rivers and lakes.

The programs are written in FORTRAN programming language to be compatible with FORTRAN77 complier. In addition, a user-friendly, menu driven program with graphics capability is developed for the IBM-PC AT computer, so that these models can be easily used to assist the oil spill clean up action in the

connecting channels should a spill occur.

This report series is organized in four volumes, to provide a complete description of the analytical formulation of the models, the logic and structures of the computer programs, and the instructions for using the models. The title of these volumes are:

Volume I: Theory and Model Formulation

Volume II: User's Manual for the River Oil Spill
Simulation Model (ROSS)

Volume III: Jser's Manual for the Lake-River Oil Spill
Simulation Model (LROSS)

Volume IV: User's Manual for the Microcomputer-Based
Interactive Program

ACKNOWLEDGEMENTS

TABLE OF CONTENTS

CHAPTER I

INTRODUCTION

In recent years there has been a growing concern over the increasing contamination of waterways and adjacent shoreline areas caused by oil spills. The Great Lakes - St. Lawrence River system (Fig. 1) is the world's largest freshwater system. Being a navigation corridor, it is subjected to the potential risk of oil contamination (Beurket and Argiroff, 1984; Argiroff and Weigum, 1986). With the possibility of oil spills in the system, an adequate means is needed for analyzing or predicting the movement and spreading of potential or accidentally spilled oil slicks. In this study, computer simulation models are developed for oil slick transport in lakes and rivers. These models can either be used on real-time basis to predict the movement of an oil spill to assist the clean up or used as scenario models to analyze possible impact of oil spills from navigation.

I.1 Fate of Oil Slicks

In order to develop an oil spill model, it is necessary to understand the transformation process of an oil slick. In addition to the location, size, and physical-chemical properties of the spill, major factors that can affect the fate of an oil slick in a water body are governed by complex inter-related transport and weathering processes. Table 1 summarizes the environmental pathways of a typical crude oil at sea. Immediately upon entering into a water body, the spilled oil

1

Figure 1. Great Lakes - St. Lawrence River System
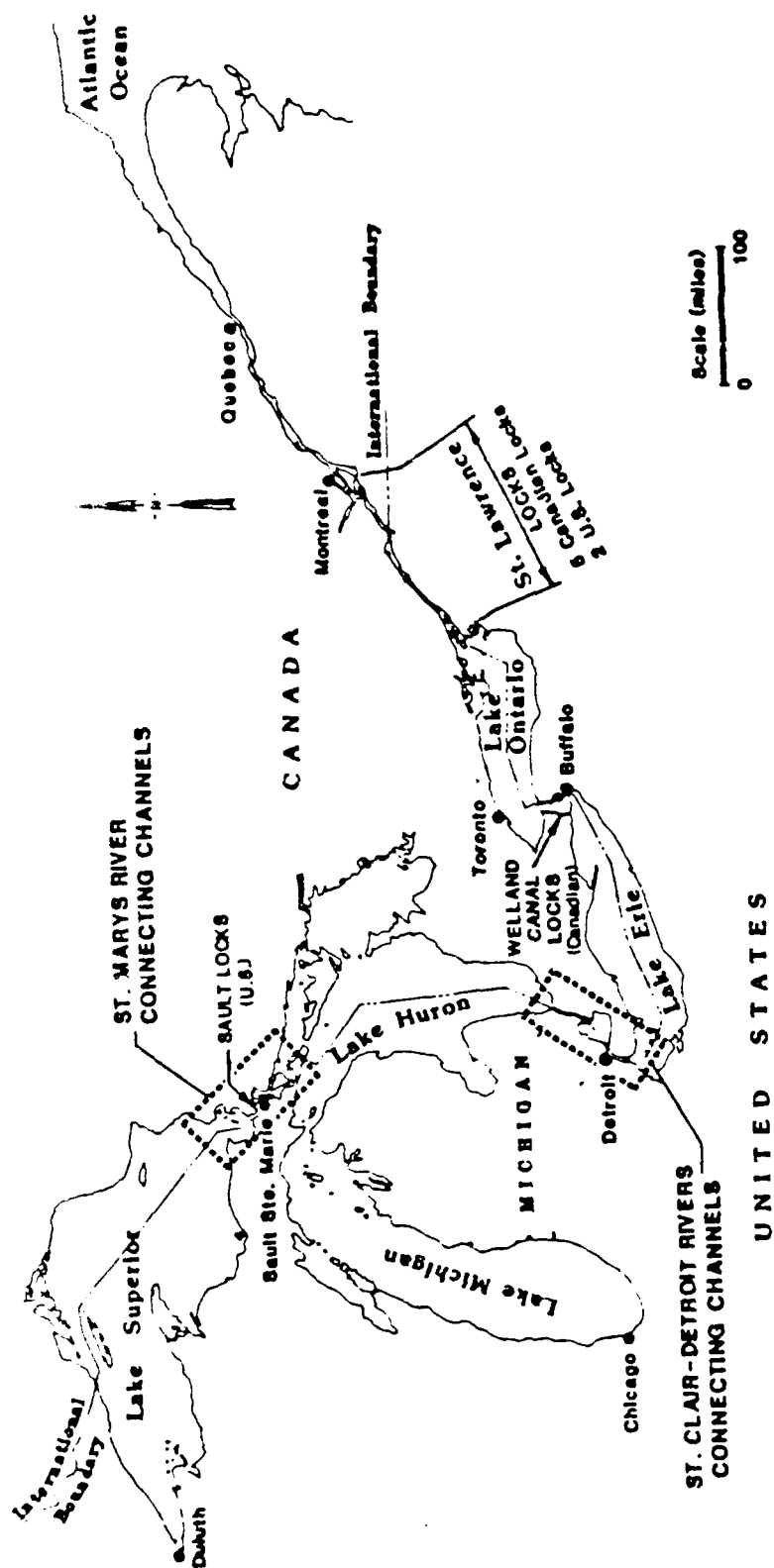
2

Table 1. Pathways for the Environmental Fate
         of Crude Oil (Butler, et al. 1976)

Pathway	Time Scale days	Percent of Initial oil
Evaporation	1 ~ 10	25
Solution	1 ~ 10	5
Photochemical	10 ~ 100	5
Biodegradation	50 ~ 500	30
Disintegration and Sinking	100 ~ 1000	15
Residue	> 100	20
TOTAL		100

spreads and forms a surface slick which covers a large area of the water surface and can be moved about by the action of winds, waves or currents. Some light hydrocarbons and some polar components begin to go into solution in the underlying water column, but most of these are lost to the atmosphere through evaporation. Evaporation of volatile components and dissolution of hydrocarbons may reduce the volume of spilled oil by as much as 50 percent during the first few days following the spill. In turbulent waters, some of the oil is emulsified into the water column as small dispersed droplets. These droplets may become dispersed because of the action of currents, or they may become attached to suspended particulate matter and slowly settle to the bottom. The turbulence action can also cause water to become entrained in the oil forming water-in-oil emulsion, which may eventually weather further forming dense tar balls. While all these are occurring, photo-chemical reactions and microbial biodegradation can also change the character of the oil and reduce the amount of oil present.

According to the above discussion, the physical and chemical processes involved in the oil slick transformation can be categorized as advection, spreading, evaporation, dissolution, emulsification, auto-oxidation, sedimentation, and biodegradation. A number of excellent reviews on these processes have been published (Jordan and Payne, 1980, Huang and Monastero, 1982, Stolzenback, et al. 1977, and Wheeler, 1978). In Fig. 2 a schematic representation of the transport and weathering processes is illustrated, along with time periods for which each of these processes are important. It is clear from

4
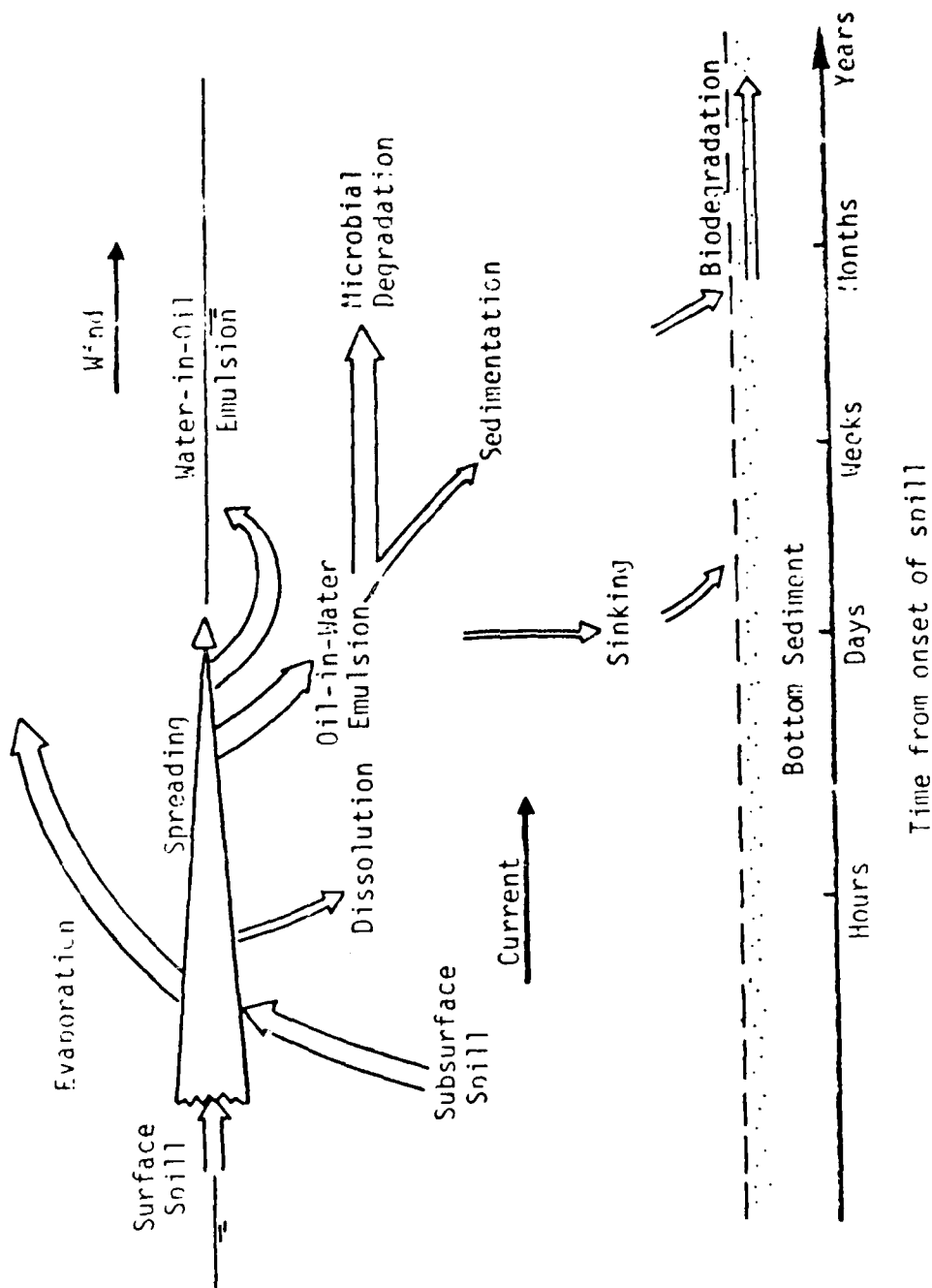
Figure 2. Physical, Chemical, and Biological Processes Affecting the Oil Slick Transformation

these time scales that the oil undergoes significant modification during the first few hours following a spill. A brief discussion of each of these physical, chemical, and biological processes follows.

Advection - Advection is a physical process which involves the drifting of the surface oil slick and the subsurface oil. The advection of surface oil is caused by the combined effects of surface current and wind drag. The advection of subsurface oil is the movement of the oil entrained in the flow due to the subsurface current.

Spreading - Spreading is another physical process which involves the areal expansion of oil slicks. The spreading process includes the mechanical spreading, and turbulent diffusion. Mechanical spreading is the spreading of the surface oil slick due to the balancing forces of inertia, gravity; viscous, and surface tension. Turbulent diffusion is the spreading of the surface oil due to the turbulent fluctuations of the wind and current velocities. Since the spreading of oil will increase the weathering processes such as evaporation, dissolution, photo-oxidation, and biodegradation, it is one of the most important porcesses affecting the fate of the spilled oil.

Evaporation - Evaporation occurs immediately after the spill. As spreading occurs more of the hydrocarbons are exposed to the atmosphere, causing evaporation rates to increase. The amount and rate of evaporation essentially depend on the percentage of light, or volatile, components in oil. Evaporation is the most significant physical-chemical process

causing the reduction in oil volume. Highly refined oils can lose 75 percent or more of its volume through evaporation within a matter of days.

Dissolution - Some oil components will be lost into the water column from a slick by dissolution. Only the low-molecular-weight hydrocarbons have an appreciable solubility in water. The fraction of oil dissolved is very small in comparison to that evaporated. However, this extraction process can be important due to the toxicity of the fraction of the oil dissolved.

Emulsification - The formation of oil-in-water emulsion is an important mode of dispersion of oil. Turbulence and wave action mix the surface layer of oil into the water column by forming many very small globules of oil which can be rapidly dispersed vertically into the water column and subject to subsurface transport. The eventual fate of oil-in-water emulsions is probably dissolution in the water column, attachment to solid particles, and biodegradation. Water-in-oil emulsions can also be formed, particuarly with heavy crudes and residual oils. The resulting emulsion contains a large pecentage of water but has a semisolid texture, often referred to as "chocolate mouses" because of their appearance. These emulsions may persist on the water surface, and disintegrate into tar lumps after a long time if not washing up on shores.

Auto-oxidation - In the presence of atmospheric oxygen, natural sunlight has sufficient energy to change the composition of the oil. This photo-oxidation process is a very slow process. The extent and rate of the photo-oxidation are

7

primarily dependent on the chemical composition of the oil and its optical density. Little is known about the effect of photochemical reactions to the overall oil slick transformation process.

Sinking/Sedimentation - Some of the spilled oil ultimately sinks if not washing up on shores. This sinking/sedimentation process occurs due to the increase in density of the oil resulting from either the evaporation and dissolution of lighter fractions of the oil or adherence onto suspended sediment. This process may eventually sink oil fractions to the bottom where they may be moved laterally, resuspended, or undergo further biological or physical-chemical reaction. Little is known about the ultimate fate of the sedimented oil.

All of the processes just described, except possibly the photo-oxidation, can only redistribute the oil. They cannot remove the hydrocarbon from the environment. Real degradation takes place only through biochemical oxidation. This biodegradation process is the principal long-term means of removing the spilled oil from the environment.

I.2 Oil Spill Simulation Models

Many of the oil spill models developed during the last decade simulate only the advection and spreading processes. Other models deal extensively with physical-chemical processes, but lack the component for simulating the advection of the slick. Only in recent models have the incorporation of both the transport and weathering processes been attempted (Huang and Monastero, 1982). Since there is a significant lack of data for

8

a reliable analytical formulation to be established for many of the weathering processes, it is impractical to include all of them into an oil spill simulation model. It would be more useful to include the most significant processes, i.e., those accounting for the bulk of the oil, while omitting others so that uncertainty in the outcome can be reduced. In addition, since part of the oil spilled in water bodies, especially in rivers and lakes, will be washed on shore, appropriate shoreline boundary conditions must also be considered in a simulation model.

Almost all of the existing oil slick models were developed for coastal marine environments. Only a few models were developed for rivers and lakes (Huang and Monastero, 1982). Tsahalis (1979) developed a simulation model for the prediction of transport, spreading, and associated shoreline contamination of oil spills in rivers. In this model, the current velocity distribution in the r.ver is calculated by empirical relationships determined from field data with some modifications for the secondary current in river bends. The oil slick is assumed to remain in circular shape with its radius calculated according to Fay's spreading laws (Fay, 1969 and 1971). The drift velocity of the slick is determined by formulas derived by Tsahalis (1979) from laboratory experiments. Fingas and Sydor (1980), developed a two-dimensional model for oil spill in rivers. In this model, the current velocity distribtuion is determined by a two-dimensional finite-difference scheme of Leendretse (1970). The entire oil slick volume is represented by a large number of individual particles. The drift velocity

9

of these particles are determined by the wind factor approach. A random fluctuation component is included to represent the horizontal diffusion. The spreading of the oil slick is calculated by Fay's spreading laws for circular slicks. For oil spills in lakes, the only model which exists is the model developed at the GLERL (Boyd, 1979, Schwab, et. al. 1984) for the Great Lakes, which is basically a model for predicting the motion of a group of surface particles. The movement of an oil slick can be simulated using this model by representing the oil slick as a group of particles. None of these three models considered the oil weathering processes. Thus the effects of weathering on the oil slick transformation cannot be accounted for.

In this study, computer models are developed for simulating the fate of oil spills in a river or a lake including the effect of ice covers. None of the previous models for oil spill in rivers and lakes took this factor into consideration. The purpose of these simulation models is to assist the on-scene-commander to develop clean up measures in the case of an actual spill and to provide assessment of likely environmental impacts of possible spills. The models are primarily designed for the prediction of the motion of an oil slick in rivers or lakes. A brief outline of the structure of the present simulation model is presetned in Fig. 3. Detailed discussions of the model formulation will be presented in Chapters II and III. In the models developed in this investigation the oil slick is considered to be composed of a large number of discrete parcels which are tracked for their

INPUT DATA

TYPE OF SPILL:	VOLUME AND TYPE OF OIL:	LOCATION AND TIME OF SPILL	RIVER/LAKE DATA:
1) Instantaneous 2) Continuous	Density, Viscosity Surface Tension, etc.		Wind Velocity Discharge and Water Levels Temperature Ice Condition

DETERMINE WATER CURRENT
-Two Dimensional Depth-Averaged
Velocity Distribution

ADVECTION

MECHANICAL SPREADING
AND
TURBULENT DIFFUSION

SHORELINE DEPOSITION

WEATHERING
(EVAPORATION, DISSOLUTION)

OUTPUT DATA

- 2D CONCENTRATION DISTRIBUTION OF OIL IN THE RIVER
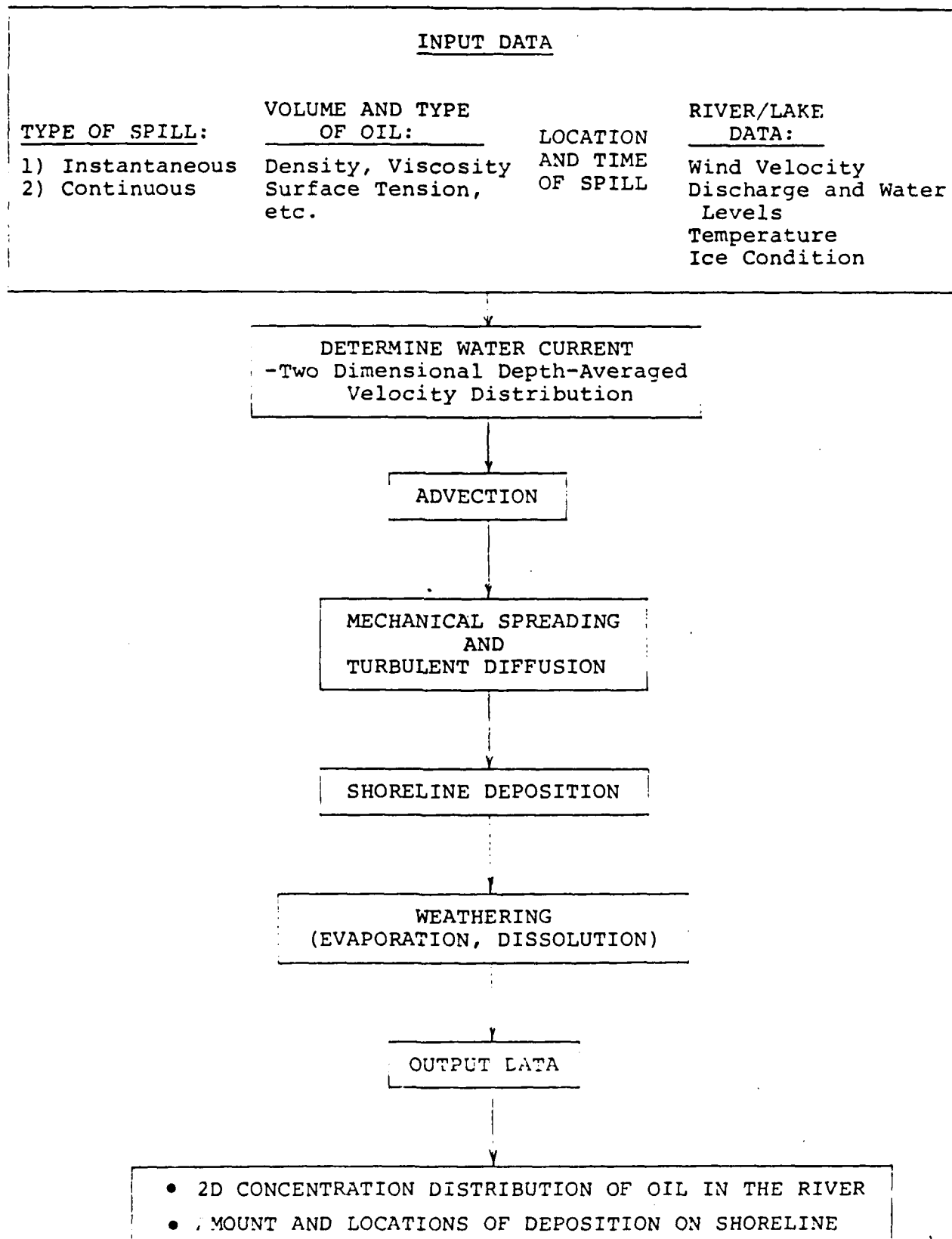- AMOUNT AND LOCATIONS OF DEPOSITION ON SHORELINE

Figure 3. Structure of the Simulation Model

11

positions and volume to each time level during the period of simulation. The two dimensional velocity distributions of the underlying river or lake water are first computed. Using the wind velocity and the computed current velocity, the advection of each parcel in the slick is determined using the wind factor approach. The spreading of the slick is simulated by considering both the mechanical spreading and surface turbulent diffusion. The model developed by Fay (1969, 1971) is used to simulate the mechanical spreading, while a random-walk simulation is used to account for the spreading due to surface turbulence. The loss of oil due to shoreline deposition is calculated according to the oil retention capability of the shoreline where the oil slick reaches. The loss of oil due to evaporation and dissolution are calculated based on empirical formulations which consider effects of slick area, wind velocity, temperature, and oil properties. As discussed in the previous sections, weathering processes which occur long after the onset of spill are not well understood and less significant. These processes are not considered in the model. This is also justified from the operational point of view, since the oil will be washed up on shore, and clean up measures will take place shortly after the spill.

The present simulation models are applied to the connecting channels of the upper Great Lakes, including the St. Mary's River, the St. Clair River, the Detroit River, and Lake St. Clair. Sample simulation results are presented in Chapter IV.

12

CHAPTER II

THEORY AND MODEL FORMULATION

II.1 The Analytical Framework

The transformation of an oil slick is affected by a number of complex physical and chemical processes. To facilitate the discussion of the model formulation, an analytical framework based on the equations of motion of a surface oil slick will first be presented. For a surface oil slick, as shown in Fig. 4, the two-dimensional depth-averaged equation of motion can be written as (Ahlstrom, 1975, Stolzenbach et. al, 1977).

$$\frac{\partial (\rho_o h)}{\partial t} + \frac{\partial (\rho_o uh)}{\partial x} + \frac{\partial (\rho_o vh)}{\partial y} = - \phi_s - \phi_b - Rh \tag{1}$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = - g(\frac{\rho_w - \rho_o}{\rho}) \frac{\partial h}{\partial x} - \frac{\tau_{bx}}{\rho h} + \frac{\tau_{sx}}{\rho h} \tag{2}$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = - g(\frac{\rho_w - \rho_o}{\rho}) \frac{\partial h}{\partial y} - \frac{\tau_{by}}{\rho} + \frac{\tau_{sy}}{\rho h} \tag{3}$$

in which x, y, and t = space and time variables; u, v = components of the oil velocity; ρ_o and ρ_w = densities of oil and water, respectively; h = oil slick thickness; g = gravity; τ_{bx} and τ_{by} = shear stress components on the bottom of the oil slick; τ_{sx} and τ_{sy} = shear stress components on the top surface
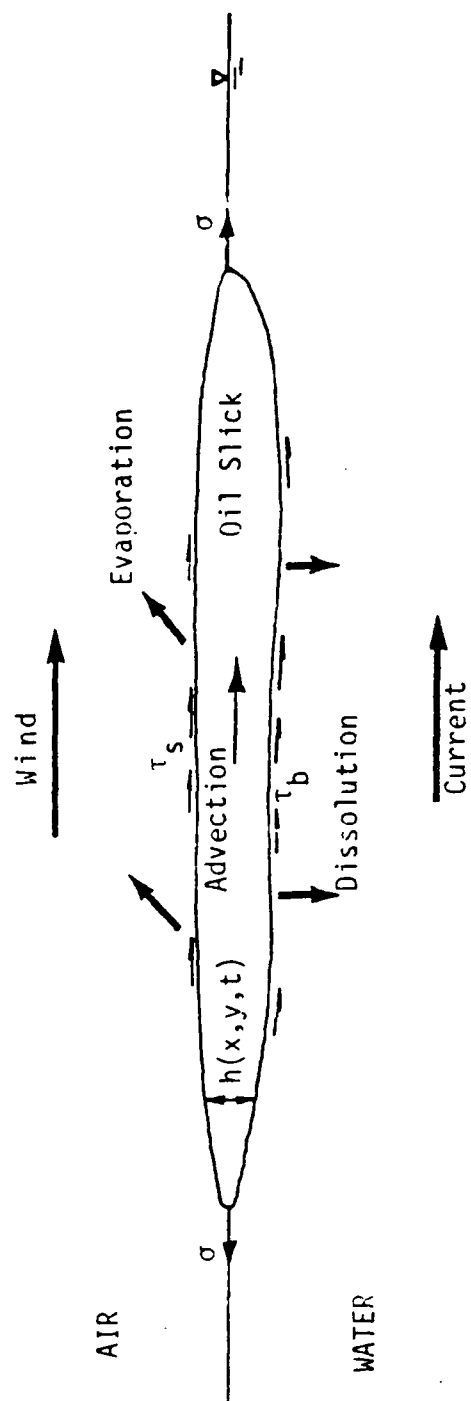
13

Figure 4. Schematic Representation of an Oil Slick

14

of the oil slick; ϕ_s = rate of oil flux outward through the top surface, e.g., evaporation; ϕ_b = rate of oil flux outward through the bottom surface, e.g., dissolution; R = other source and sink terms. The density of oil can be determined from its specific gravity. Typical values of the specific gravity are: 0.7 for gasoline, 0.8 for kerosene,. 0.84 for Diesel or No. 2 fuel oil, and 0.98 for Bunker C or No. 6 fuel. The specific gravity of crude oils varies between 0.80 and 0.99 (Bishop, 1983). The boundary condition at the circumference of the slick, is that the force parallel to the water surface and normal to the slick boundary, f_n, be balanced by the net surface tension force, i.e.,

$$f_n = \sigma = \sigma_{aw} - \sigma_{oa} \cos\theta_{oa} - \sigma_{ow} \cos\theta_{ow}$$
$$\cong \sigma_{aw} - \sigma_{oa} - \sigma_{ow} \tag{4}$$

where σ_{aw} = surface tension of air-water interface, 72.75 dynes/cm at $20^\circ C$; σ_{oa} = surface tension of air-oil surface, 20 dynes/cm for many crudes; σ_{ow} = surface tension of oil-water interface, varies between 15 and 25 dynes/cm (Stolzenbach, et al. 1977). Eqs. 1 to 4 clearly show that the movement of an oil slick is governed by the advection due to the viscous forces acting on the top and bottom surfaces of the slick, the spreading due to gravitational, viscous, and surface tension forces, and the changes in the mass and physical-chemical properties of the oil due to various weathering processes.

A number of studies have attempted to analyze in detail the hydrodynamic problem defined above (Kerr and Babu, 1970;

15

DePietro and Cox, 1979; and Foda and Cox, 1980). These complex mathematical treatments are not suitable for applications to real field problems. In the present study, a Lagrangian discrete-parcel algorithm is used. In this algorithm the oil slick is viewed as a large ensemble of small parcels. Each parcel has associated with it a set of spatial coordinates, and a specific quantity of mass. The movement of each parcel in the river or the lake is affected by the wind, water current, and the concentration of surrounding parcels. If a large number of such parcels are released in a water body, and their discrete path and mass are followed and recorded as functions of time relative to a reference grid system fixed in space, then the density distribution of the ensemble in the water body can be interpreted as the concentration of the oil. The approach requires an efficient book-keeping procedure rather than the solution of a large matrix associated with a conventional Eulerian finite-difference or finite-element methods. The algorithm is inherently stable with respect to time steps although the time step should be compatible with the grid size and velocity for numerical accuracy (Cheng, et al. 1984). Since the movement of each parcel in the oil slick is dependent upon the distribution of the entire ensemble, all parcels must be traced to each time level before proceeding to the next.

The detailed structure and implementation of the present numerical model will be discussed and presented in Chapter III. In the following sections the analytical formulations used for each component of the model will be discussed.

II.2 **River Current Simulation**

Since the water current affects both the advection and the
spreading of an oil slick, it is necessary that the distribution
of both the magnitude and the direction of the current be
determined first.   Numerous numerical methods exist in the
literature for determining the two-dimensional flow distribtuion
in shallow waters (Leendretse, 1970; Grubert, 1976; Hamilton, et
al. 1982).   However, due to the stability and accuracy problems
of the numerical method, the geometric element size, A_e, and the
size of time steps t, are limited by   t $\leq$ $(A_e/gh)^{1/2}$.   This
makes the use of this type of method impractical for long
rivers.   In view of the need for simulating flow distribution in
long river reaches, an alternative approach is taken in the
present study.   In the present approach, the time-dependent
discharge distribution Q(x,t) along the river is first obtained
through the use of a one-dimensional hydraulic transient model
(e.g. Thomas, 1984), which was developed based on the St.Venant
equations:

$$\frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = 0 \tag{5}$$

$$\frac{\partial Q}{\partial t} - \left(\frac{Q}{A}\right)^2 \frac{\partial A}{\partial x} + \frac{2Q}{A} \frac{\partial Q}{\partial x} + gA \frac{\partial H}{\partial x} - gA(S_o - S_f) = 0 \tag{6}$$

in which, x = longitudinal distance along the river; A = flow
cross-sectional area; H = water level; S_o = bed slope; and S_f =
frictional slope. The friction slope can be calculated by
Manning's equation.

17

$$S_f = \frac{n_b^2 Q^2}{2.21 A^2 R^{4/3}} \tag{7}$$

in which, R = hydraulic radius, and n = the Manning's roughness coefficient of the bed. For an ice-covered reach, the composite Manning's coefficient, which accounts for the resistance of ice cover and the river bed, should be used insteady of n_b. The composite Manning's coefficient can be calculated by the Belokon-Sabaneev formula.

$$n = [\frac{1}{2} (n_i^{3/2} + n_b^{3/2})]^{2/3} \tag{8}$$

The hydraulic radius can be assumed to be half of the flow depth for ice-covered reaches.

Once the one-dimensional solution is obtained, the discharge Q can then be distributed across the width of the river using a stream-tube model (Shen and Ackermann, 1980), to give the two-dimensional velocity distribution at selected cross sections.

<u>Two-Dimensional Velocity Distribution</u> — For any channel cross-section, as shown in Fig. 5, the transverse distribution of the flow can be determined using a simplified method developed by Shen and Ackermann (1980). In this method, the cross-section is first discretized into trapezoidal elements. By applying Manning's equation to the ratio of discharges between the entire cross section and a partial cross section (Fig. 5), the following expression can be written:
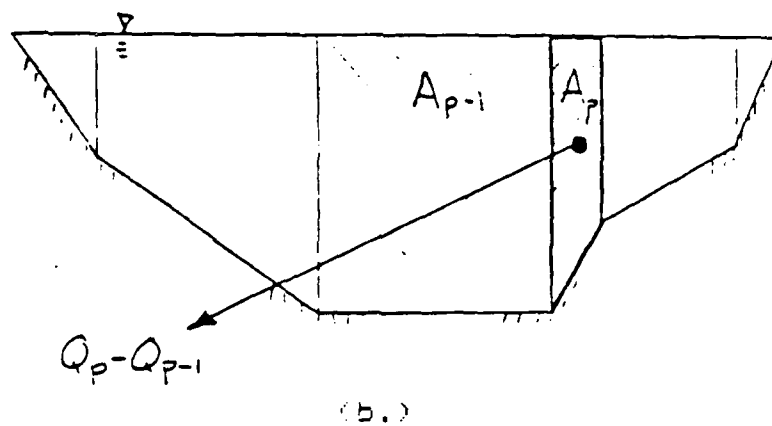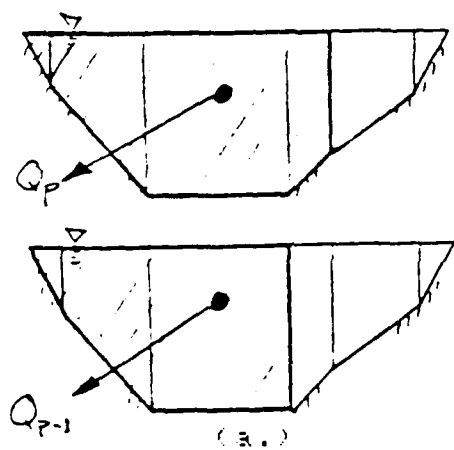
18

Figure 5. a) Cumulative discharges over a partial cross section;
           b) Area and discharge through p^{th} trapezoid.

$$\frac{Q_P}{Q} = \frac{\sum_{p=1}^{P} A_p R_p^{2/3}}{\sum_{n=1}^{N} A_n R_n^{2/3}} \qquad (9)$$

where, P = number of trapezoids in the partial cross section; N = total number of trapezoids describing a cross section geometry; Q_P = cumulative discharge up to and including the pth trapezoid; Q = the total discharge through the entire cross section; A_n and R_n = area and hydraulic radius, respectively, for the nth trapezoid; and A_p and R_p = area and hydraulic radius of the pth trapezoid, respectively.

The cumulative discharge, Q_P, can be computed by first rewriting Eq. 9 as:

$$Q_P = F_Q \sum_{p=1}^{P} (A_p R_p^{2/3}) \qquad (10)$$

with

$$F_Q = \frac{Q}{\sum_{n=1}^{N} (A_n R_n^{2/3})} \qquad (11)$$

and

$$Q_P - Q_{P-1} = F_Q A_p R_p^{2/3} \qquad (12)$$

Based on the computed distribution of Q_P, stream-tube boundaries within the cross section can be determined by simple interpolation. Once the stream-tube boundaries are located, the flow through each stream-tube is then divided by the cross sectional area of the stream-tube to obtain the depth-averaged

20

velocity.

$$V_p = Q_s/A_s \qquad (13)$$

This velocity is then assigned to the center of the stream-tube. By applying the above procedure to successive cross sections along the river, a two-dimensional depth-averaged velocity distribution can be obtained. The directions of velocity vectors are the same as the vector connecting center points of each streamtube at successive cross sections. As an example, the simulated depth-averaged velocity distribution for a reach of the St. Clair River is shown in Fig. 6.

Once the velocity distribution along stream-tubes is established, the distribution of velocity for all the points in a predefined grid system, as shown in Fig. 7, can be obtained through linear interpolations. Calculated velocities are found to compare favorably with data obtained in the field (U.S. Army Corps of Engineers, 1974).

II.3 Lake Circulation

The following equations of motion describe the circulation in shallow lakes, if nonlinear convective terms are neglected.

$$\frac{\partial M}{\partial t} - fN = - gD \frac{\partial H}{\partial x} + \frac{1}{\rho_w} (\tau_x^s - \tau_x^b - \tau_x^i) \qquad (14)$$

$$\frac{\partial N}{\partial t} + fM = - gD \frac{\partial H}{\partial y} + \frac{1}{\rho_w} (\tau_y^s - \tau_y^b - \tau_y^i) \qquad (15)$$

and $\frac{\partial H}{\partial t} + \frac{\partial M}{\partial x} + \frac{\partial N}{\partial y} = 0$ \qquad (16)
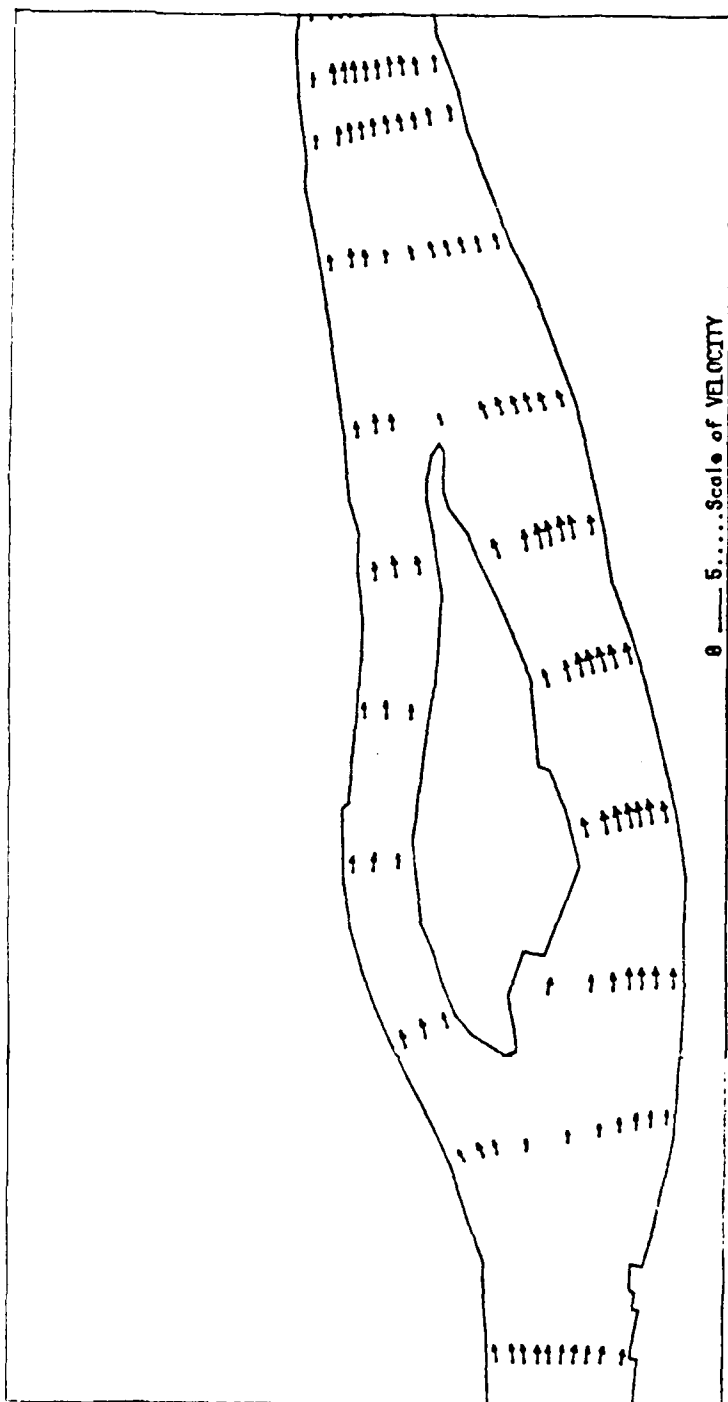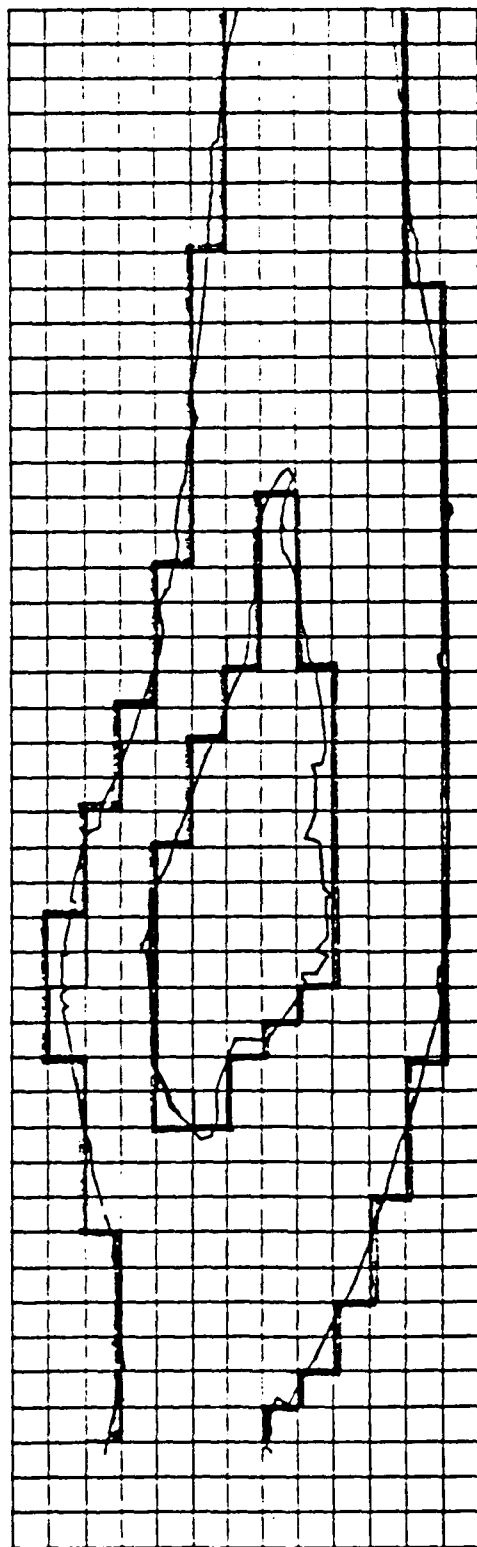
21

Figure 6. Velocity Distribution in Stream Tubes

Grid Size: 500 x 500 ft^2

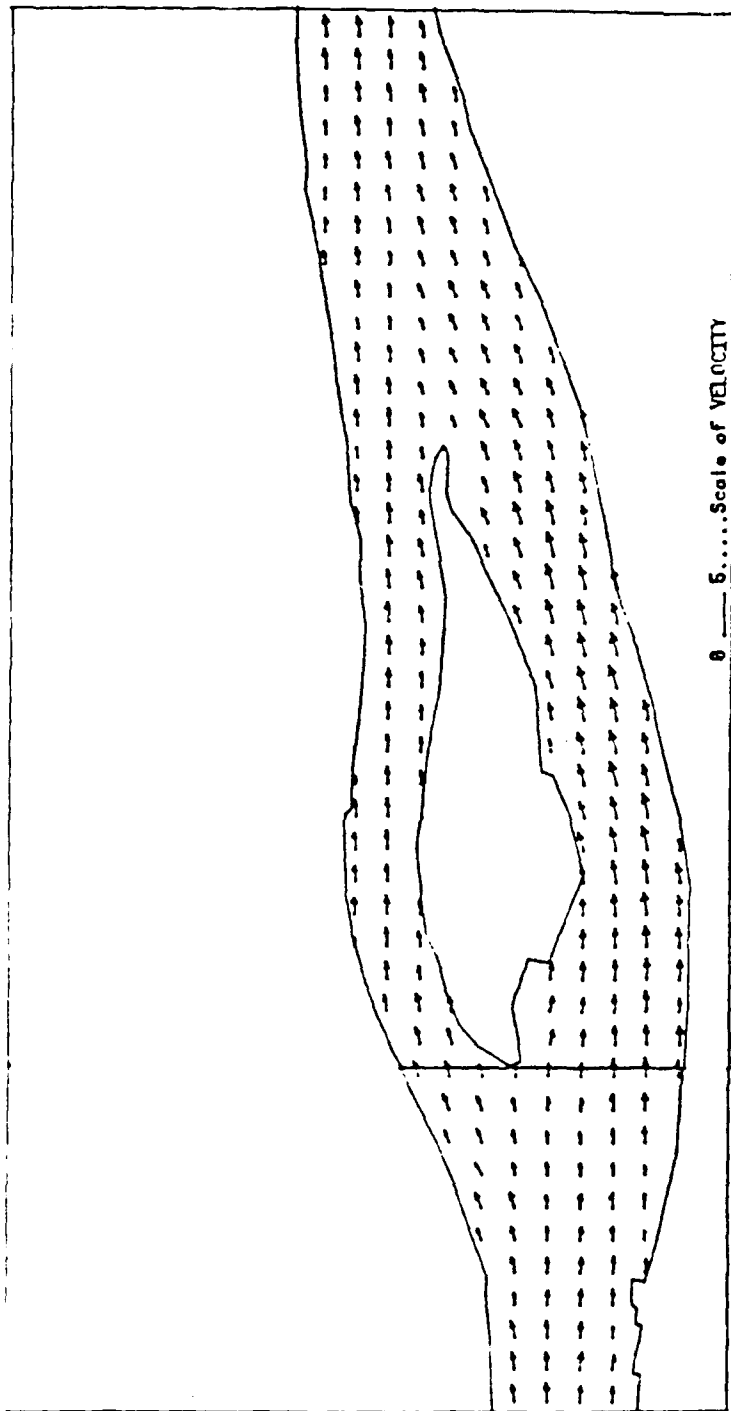Figure 7a. A River Reach with Superimposed Grid System

Figure 7b. Velocity Distribution on the Grid System

24

in which, $M = u_c D$ and $N = v_c D$ in which, u_c and v_c = depth-average velocity components; D = depth of the flow; H = water surface elevation; g = gravity; $f = \Omega \sin\phi$, coriolis parameter; Ω = angular velocity of the earth; ϕ = latitude; τ_x^s, τ_y^s = components of the wind stress; τ_x^b, τ_y^b = components of the bed shear; τ_x^i, τ_i^y = components of shear stress at the ice-water interface; and x, y, t = space and time variables. For simulating the circulation pattern in the Lake St. Clair, the RLID finite difference model developed by Schwab, et. al (1981) is used. In this model, the free surface fluctuation is neglected. Eq. 16 then leads to the existence of the stream function ψ, defined by

$$M = -\frac{\partial \psi}{\partial y} \quad , \quad N = \frac{\partial \psi}{\partial x} \tag{17}$$

Combining this with Eqs. 14 and 15, will yield:

$$\frac{\partial}{\partial t}(\nabla \cdot D^{-1}\nabla\psi) + f\left(\frac{\partial \psi}{\partial x}\frac{\partial D^{-1}}{\partial y} - \frac{\partial \psi}{\partial y}\frac{\partial D^{-1}}{\partial x}\right) \tag{18}$$

$$= \frac{\partial}{\partial x}\left(\frac{\tau_y^s - \tau_y^b - \tau_y^i}{D\rho_w}\right) - \frac{\partial}{\partial y}\left(\frac{\tau_x^s - \tau_x^b - \tau_x^i}{D\rho_w}\right)$$

Eq. 18 is used to solve for ψ values through a second-order finite difference scheme. The velocity distribution is determined from the calculated ψ values. A sample result for velocity distribution in the Lake St. Clair is shown in Fig. 8.

II.4 Advection

Advection in Open Water

Advection or drifting of oil on the water surface is the
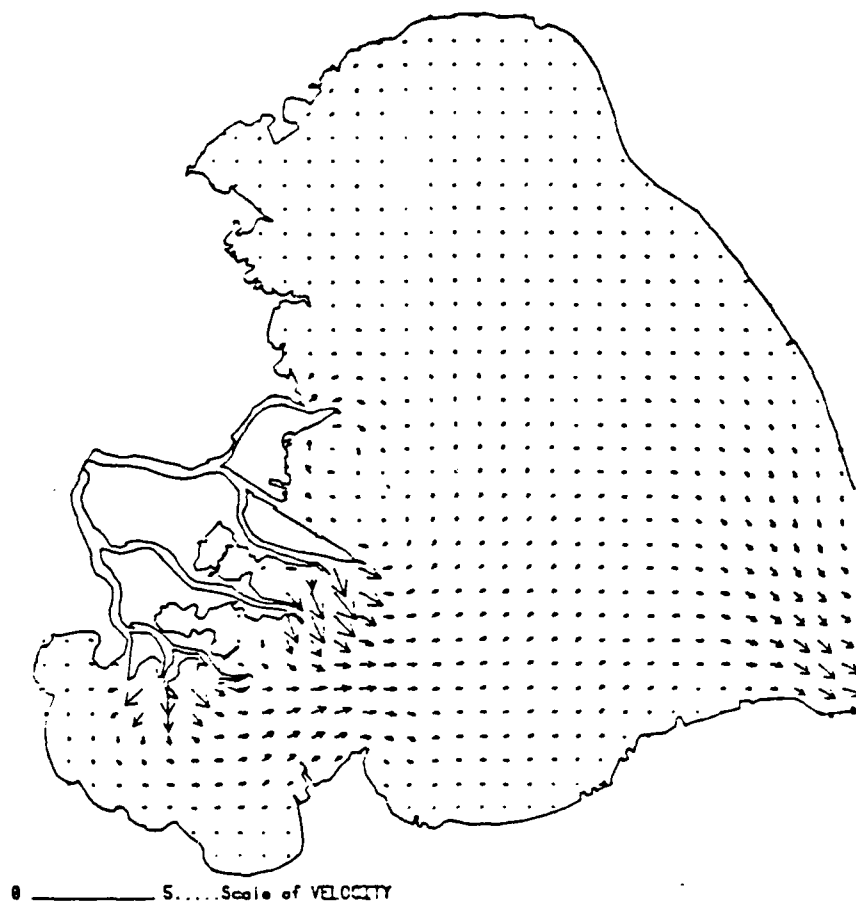
25

Figure 8.   Velocity distribution in Lake St. Clair,
            Stage and discharge at the outlet of the
            lake are 573.72 ft. and 18416 cfs, respectively.

result of the combined action of wind, current and wind generated waves (Schwartzberg, 1971, Tsahalis, 1979). The drift velocity of the surface oil is usually considered to be a vector sum of a wind induced drift and a water current induced drift (Stolzenback, et al. 1977). In the present model the advective velocity of each oil parcel is computed as:

$$\vec{V}_t = \vec{V} + \vec{V}'$$
(19)

in which $\vec{V}_t$ = drift velocity of an oil parcel; $\vec{V}$ and $\vec{V}'$ = the mean and turbulent fluctuation components of the drift velocity. The component $\vec{V}'$ is included to simulate the horizontal diffusion of the oil parcels. The formulation for $\vec{V}'$ will be discussed later in this section. The mean velocity component $\vec{V}$ includes both the wind and water current effects, and can be calculated by the formula.

$$\vec{V} = \alpha_w \vec{V}_w + \alpha_c \vec{V}_c$$
(20)

in which $\vec{V}_w$ = wind velocity at 10 meters above the water surface, $\vec{V}_c = \vec{u}_c + \vec{v}_c$ = depth-averaged current velocity, α_w = wind drift factor to account for the drift of surface slick due to wind effect; and α_c = a factor to account for the contribution of the drift of the oil slick at the water surface due to the current.

Wind induced surface currents have been reported to vary between 1% and 6% of the wind speed with 3% being the most widely used drift factor in oil slick trajectory models

27

(Stolzenbach, et al., 1977). Based on Madsen's (1977) Ekman layer model, a drift factor of 0.03 can also be obtained with appropriate values of equivalent roughness height of the free surface (Huang and Monastero, 1980).

Assuming a logrithmic velocity profile, the surface velocity of the water current can be related to the depth-averaged current velocity by the relationship

$$\frac{V_s}{V_c} = 1 + \frac{u_*}{KV_c} \tag{21}$$

in which, V_s = surface velocity; u_* = shear velocity, and k = Karman constant, 0.4. Calculations based on conditions in the connecting channels, the ratio V_s/V_c is found to vary between 1.1 and 1.2 with most of the values equal to 1.1. In the present simulation, values of 0.03 and 1.1 are used for α_w and α_c, respectively.

Advection Under Ice Cover

Oil spilled under ice is a topic which has received little theoretical or laboratory treatment. As suggested by the experimental study of Cox and Schultz (1981), an ice cover may be classified into three categories when determining slick advection. The ice cover may be smooth, contain small roughness elements, or contain large roughness elements. The following discussion summarizes the results of limited experimental studies and serves as the basis for modeling the advection of oil in the present simulation.

Under smooth ice covers with no current, the oil will rest

28

at an equilibrium thickness which is described by the empirical
equation:

$$\delta_{eq} = 1.67 - 8.5(\Delta\rho_w) \qquad (22)$$

where δ_{eq} = the static equilibrium slick thickness, cm; $\Delta = (\rho_w - \rho_o)/\rho_w$, the relative density difference between oil and water; and ρ_w and ρ_o = the water and oil densities in the unit of gm/cm^3, respectively. An ice cover is considered to be smooth when the height of the ice roughness is smaller than the equilibrium thickness of the oil, δ_{eq}.

The depth-average current velocity at which the oil just begins to move along an ice cover is called the threshold velocity, U_{th}. For a smooth cover, the value of U_{th} was empirically determined to be a function of the oil viscosity, μ_o, and is given as:

$$U_{th} = 305.79/(88.68 - \mu_o) \qquad (23)$$

where U_{th} has the unit cm/sec and μ_o has the unit g/cm-sec. Viscosities for crude and fuel oils fall in the range of 5 to 50 centipoises (1 cp = 1.0 x 10^{-2} gm/cm-sec or 1 cp = 2.4 lb/ft-hr). Typical values of oil viscosity can be found in fluid mechanics books (e.g. Rouse, 1946).

A rough ice cover has the ability of retaining the oil between the roughness elements. As the current velocity is increased, the oil will creep along the upstream face of the roughness element until it spills over the element and moves

29

downstream. The threshold current velocity at which the oil will move downstream under a rough ice cover is called the failure velocity, U_{fl}.

$$U_{fl} = 1.5 \left\{ 2 \left(\frac{\rho_o + \rho_w}{\rho_o \, \rho_w} \right) \left[\sigma_{o/w} g (\rho_w - \rho_o) \right]^{1/2} \right\}^{1/2} \tag{24}$$

where $\sigma_{o/w}$ = the oil water inerfacial tension. The failure velocity U_{fl} is the velocity above which no oil can be contained upstream of a large roughness element.

If the depth-averaged ᐸurrent velocity is less than the threshold velocity, the slick will not advect. If the depth-averaged velocity is greater than the threshold velocity, U_{th} or U_{fl}, the relationship between the current velocity and the slick velocity is given as:

$$\left(1 - \frac{V}{V_c} \right)^2 = \frac{K}{0.115 \, F_\delta^2 + 1.105} \tag{25}$$

with

$$F_\delta = \frac{V_c}{\sqrt{\Delta g \delta_{eq}}} \tag{26}$$

where V = the mean drift velocity; V_c = the current speed; K = the friciton amplification factor; F_δ = the slick densimetric Froude Number; and g = gravitational acceleration. The value of K is a function of the roughness height of the cover. With the limited data available, K is assumed to vary linearly between 1.0 for a smooth cover and 2.6 for an ice cover with Manning's

30

roughness coefficient $n_i = 0.055$.

Horizontal Diffusion

The term V' in Eq. 19 is included to account for the horizontal diffusion due to the turbulent fluctuation of the drift velocity. For isotropic turbulent diffusion, the diffusion coefficient E_T can be related to the magnitude of V' by the random walk analysis (Fischer, et al., 1979), where

$$V' = (4E_T/\delta t)^{1/2} \tag{27}$$

in which δt = time step. Murray (1972) using the Fickian diffusion theory estimated the value of diffusion coefficient for the 1970 Chevron spill to be 19 m^2/sec. Cole, et al. (1973) used a value of 4.5 ft^2/sec, based on dye tests for the simulation of oil spill at Cherry Point Refinery in the Straight of Georgia. Hunter (1980), by fitting observed spreading of oil slicks to Okubo's (1968) theory, suggested a value of a 5 m^2/sec. All of these analyses were based on coastal oil spills. In rivers and shallow lakes, the diffusivity will be affected by the shear velocity, u_*, and the depth of flow, D, in addition to the wind condition. Flume experiments by Sayre and Chang (1969) indicated that E_T is in the order of 0.6 Du_*. This expression may be used to calculate the turbulent diffusion in rivers. For lakes, the following formula for surface dye patches (Okubo, 1962) may be used.

$$E_T = 0.0027 \, t^{1.34} \tag{28}$$

31

In this equation the units for E_T and t are cm^2/sec and second, respectively.

In the present simulation, the fluctuation velocity component $\vec{V}'$ is calculated by

$$\vec{V}' = V' R_n e^{i\theta'} \qquad (29)$$

For a selected E_T value the magnitude of V' is computed using Eq. 27. R_n is a normally distributed random number with a mean value of 0 and a standard deviation of 1. The directional angle θ' is assumed to be a uniformly distributed random angle ranging between 0 and π.

During each time step Δt, the displacement, ΔS, of each oil parcel is calculated by numerically integrating the drift velocity $\vec{V}_t$ over the time period Δt. When the Δt value is large, subintervals δt_k are used for the advection of oil parcels, for numerical accuracy. In this case, the displacement during the time interval t is

$$\Delta \vec{S} = \sum^{k} \vec{V}_k \, \delta t_k \qquad (30)$$

in which, $\vec{V}_k$ = drift velocity of an oil parcel during the time interval δt_k, $\Delta \vec{S}$ = displacement during the time interval Δt, and $\sum^{k} \delta t_k = \Delta t$. The values of δt_k should satisfy the condition (Roache, 1968 and Cheng, et al., 1984)

$$\delta t_k \leq [\frac{u_k}{\Delta x} + \frac{v_k}{\Delta y}]^{-1} \qquad (31)$$

in which, u_k and v_k are the x and y components of the velocity V_k.

II.5 Mechanical Spreading

Spreading in Open Water

Spreading of the oil slick is one of the most important processes in the early stage of the oil slick transformation, because of the influence of the surface area of the oil slick on weathering processes such as evaporation and dissolution. Besides the horizontal dispersion due to advection, and turbulent diffusion, the spreading of an oil slick is determined by the balance of gravitational, viscous, and surface tension forces. The spreading is also affected by weathering processes which tend to change the mass and physical-chemical properties of the oil slick.

Several models have been proposed for the process of mechanical spreading in open water (Fay 1969, 1971; Hoult, 1972; Blokker, 1964; and Mackay, et al. 1980). In this study, Fay's spreading theory (1971) is used for the reason that this theory is based on a rather comprehensive description of the spreading mechanisms and has been verified by laboratory experiments (Fay, 1971; Hoult and Suchon, 1970) and other analytical solutions (Fannelop and Waldman, 1971).

Fay's spreading theory is derived for single component, constant volume slicks with idealized configurations in quiesent water. This theory considered the spreading of oil as a result of two driving forces, gravity and surface tension, counterbalanced by the retarding forces of inertia and viscosity. The spreading of an oil slick is considered to pass through three phases. In the beginning phase, only gravity and inertia forces are important. In the intermdediate phase the

33

gravity and viscous forces dominate. In the final phase the surface tension is balanced by viscous forces. Formulas for both the one-dimensional spreading and the radial spreading at different stages are summarized in Table 2.

The spreading rate during each phase can be obtained by taking time derivatives of the formulas given in Table 2. The equations for spreading rates are summarized in Table 3. The time rate change of the oil volume in these equations represent the change due to weathering and the changes in oil volume distribution in various parts of the slick. In addition to the rates of spreading at different phases, the times at which each phase transition occurs also need to be determined. These transition times can be obtained by letting equations in the appropriate phases equal to each other and solving for the time. Equations for the transition times are summarized in Table 5. Fay (1969, 1971) observed that the changes in slick properties caused by weathering may result in the eventual cessation of the mechanical spreading. Based on a number of field observations, Fay suggested that

$$A_f = 10^5 \, \forall^{3/4} \tag{32}$$

in which A_f = the final slick area in m^2, and V = total volume of the slick in m^3. In this study the cessation of the mechanical spreading is considered to occur when the s⌐⌐ck thickness reduces to $10^{-5} \, \forall^{1/4}$ meter. To illustrate the respective regimes of the different phases of spreading, variations of the radius and thickness of circular slicks of

34

Table 2.   Spreading Laws for Oil Slicks

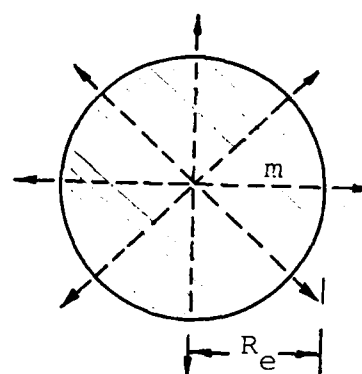(Fay,   1971; Houlc, 1972; and Waldman, et al., 1973)
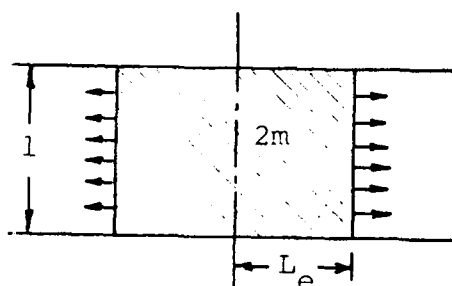
One-Dimensional   Axisymmetric

mass, $m = \rho_o L^2 \times 1$ mass, $m = \rho_o L^3$

volume $= L^2 \times 1 = A \times 1$ volume $= L^3 = \forall \times 1$

Spreading Phase	L_e (1-Dimensional)	R_e (Radial)
Gravity-Inertia	$1.39(\Delta g A t^2)^{1/3}$	$1.14(\Delta g \forall\, t^2)^{1/4}$
Gravity-Viscous	$1.39(\Delta g A^2 t^{3/2} \nu^{-1/2})^{1/4}$	$0.98(\Delta g \forall^2 t^{3/2} \nu^{-1/2})^{1/6}$
Surface Tension Viscous	$1.43\ (\sigma^2 t^3 \rho_w^{-2} \nu^{-1})^{1/4}$	$1.60(\sigma^2 t^3 \rho_w^{-2} \nu^{-1})^{1/4}$

$\Delta = 1 - (\rho_o/\rho_w)$, $\nu = \nu$ of water

Table 3. Spreading Rates of Oil Slicks and Phase Transition Times

A. Spreading Rates for One-Dimensional Slicks, dL_e/dt.

Spreading Phase	Spreading Rate
Gravity-Inertia	$(\Delta g)^{1/3}(L^{-1/3}\frac{dL}{dt}t^{2/3} + L^{2/3}t^{-1/3})$
Gravity-Viscous	$1.39(\Delta g\nu^{-1/2})^{1/4}(\frac{3}{8}Lt^{-5/8} + \frac{dL}{dt}t^{3/8})$
Surface Tension-Viscous	$1.43(\sigma\rho_w^{-1})^{1/2}(\frac{3}{4}t\nu)^{-1/4}$

$^*L^2$ = volume of oil per unit length along the major axis of the slick, (L is a characteristic length)

B. Spreading Rates for Circular Oil Slicks, dR_e/dt.

Spreading Phase	Spreading Rate
Gravity-Inertia	$0.285(\Delta g)^{1/4}(t^{1/2}\forall^{-3/4})(\frac{d\forall}{dt} + \frac{2\forall}{t})$
Gravity-Viscous	$0.98(\Delta g\nu^{-1/2})^{1/6}(\frac{1}{3}\forall^{-2/3}t^{1/4}\frac{d\forall}{dt} + \frac{1}{4}\forall^{1/3}t^{-3/4})$
Surface Tension-Viscous	$1.20(\sigma^2\rho_w^{-2}\nu^{-1}t^{-1})^{1/4}$

$^*\forall$ = Total volume of the slick

C. Times of Phase Transition

Transition	One-Dimensional Spreading	Radial Spreading
Gravity-Inertia to Gravity-Viscous	$(L^8\nu^{-3}\Delta^{-2}g^{-2})^{1/7}$	$0.55(\forall\nu^{-1}\Delta^{-1}g^{-1})^{1/3}$
Gravity-Viscous to Surface Tension-Viscous	$(0.89\Delta gL^4\sigma^{-2}\rho_w^2\nu^{1/2})^{2/3}$	$0.38(\rho_w/\sigma)(\Delta g\nu\forall^2)^{1/3}$

different volumes resulting from an instantaneous spill are presented in Figs. 9 and 10. Phase transitions are indicated by circles in these figures.

Formulas presented in Tables 2 and 3 were drived for simple slick geometries that exist under idealized conditions. In the simulation model, the radial spreading formulas are used when the slick is nearly circular, and the one dimensional formulas are used when the slick area is in elongated shape. A slick is considered to be elongated when the aspect ratio of the slick area is greater than 3.

The aspect ratio refers to the length to width proportion of the slick and the orientation refers to the angle, θ, the major axis of the slick makes with the x axis, as shown in Fig. 11.

The orientation of the slick is computed using the moments and the product of inertia of the slick. The angle, θ, can be expressed using:

$$\tan (2\theta) = \frac{-2P_{xy}}{I_x - I_y} \tag{33}$$

where

$$I_x = \Sigma y^2 \ , \ I_y = \Sigma x^2 \ , \ P_{xy} = \Sigma xy \tag{34}$$

in which I_x and I_y are the moments of inertia of the oil slick with respect to the x and y axis respectively and P_{xy} is the product of inertia. Once the orientation is known, the x and y coordinates of all the particles in the slick are transformed
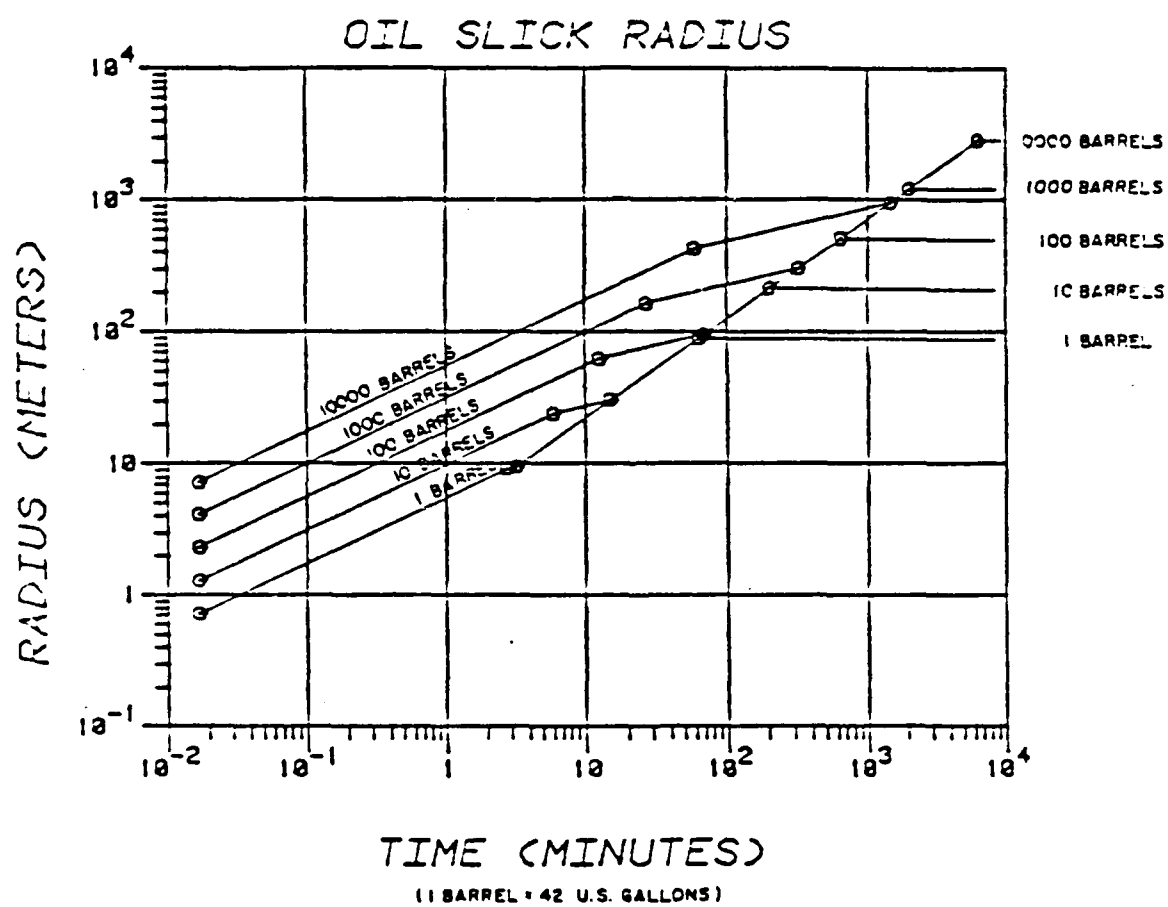
37

Figure 9. Plot of slick radius versus time, $\rho_w = 1.09 m/cm^3$, $\rho_o = 0.9 gm/cm^3$, $\nu_w = 2.543 \times 10^{-2}$ cm^2/sec, $\sigma = 11.02$ dynes/cm.
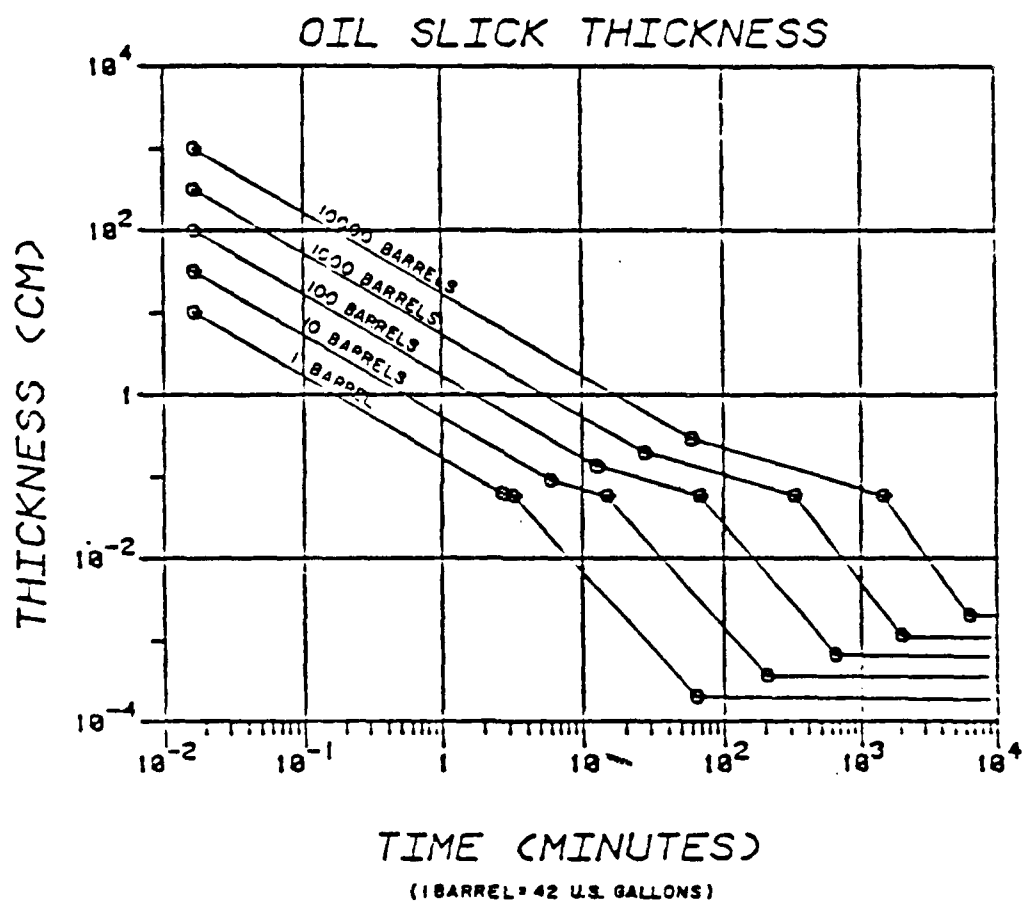
OIL SLICK THICKNESS

Figure 10.   Plot of slick thickness versus time, $\rho_w = 1.0$ gm/cm^3, $\rho_o = 0.9$ gm/cm^3, $\nu_w = 2.543 \times 10^{-2}$ cm^2/sec, $\sigma_o = 11.02$ dynes/cm.
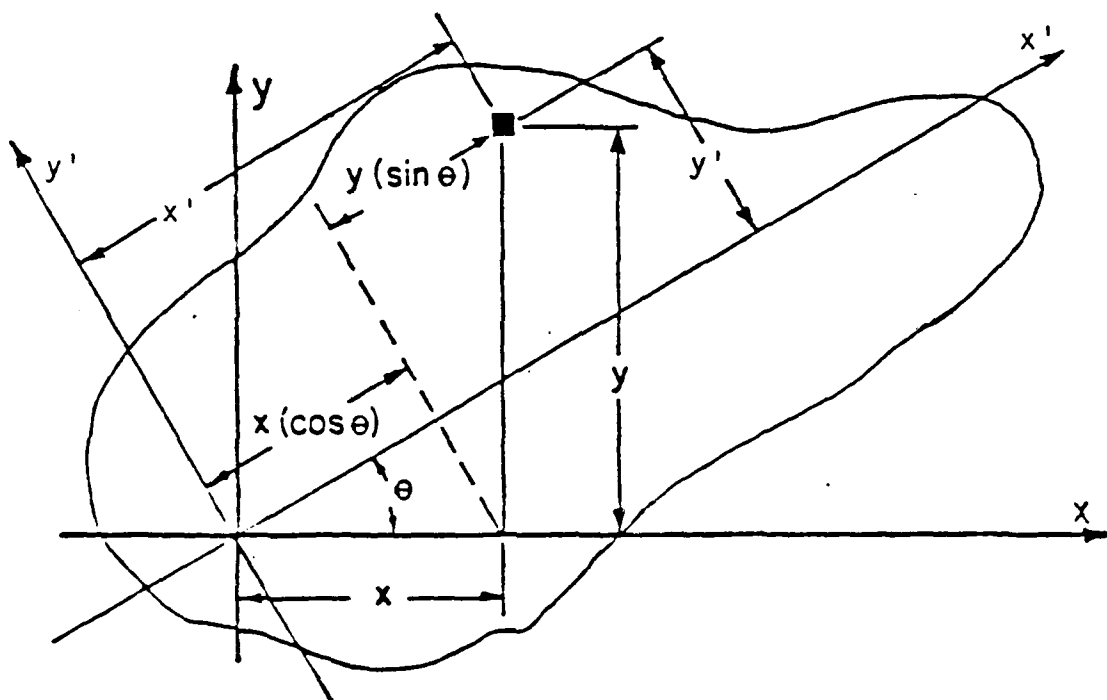
Figure 11. Definition sketch for variables used to compute slick aspect ratio and orientation

into coordinates in a x', y' coordinate system in which the x' axis is the major axis of the slick. The aspect ratio is computed by Eq. 35 based on the x', y' coordinates of all the oil particles.

$$\text{Aspect Ratio} = \frac{\Sigma x'}{\Sigma y'} \tag{35}$$

This aspect ratio is used to determine whether the spreading of the oil slick is radial or one-dimensional. The use of 3.0 for the aspect ratio at the transition from radial spreading to one-dimensional spreading is a subjective estimate, but gives reasonable results.

For a nearly circular slick, the slick area is divided into eight pie-shaped sectors as shown in Fig. 12. For an elongated slick, the entire slick is broken up into a series of strips of finite width of the same order as the grid size as shown in Fig. 13. For both cases, the spreading rate of each segment is calculated using Fay's formula independent of other segments in the slick. This simplification inherently assumed that concentration gradients at the boundaries between neighboring segments are negligible for mechanical spreading. The segmentization also allows for different spreading rates in different regions of the slick, thus providing a more realistic description of the field situation. During each time step the increase in mean radius of each pie-shaped sector in a nearly circular slick or the mean width of each segment in an elongated slick due to the mechanical spreading can be calculated from the spreading formulas given in Table 3. For a nearly circular
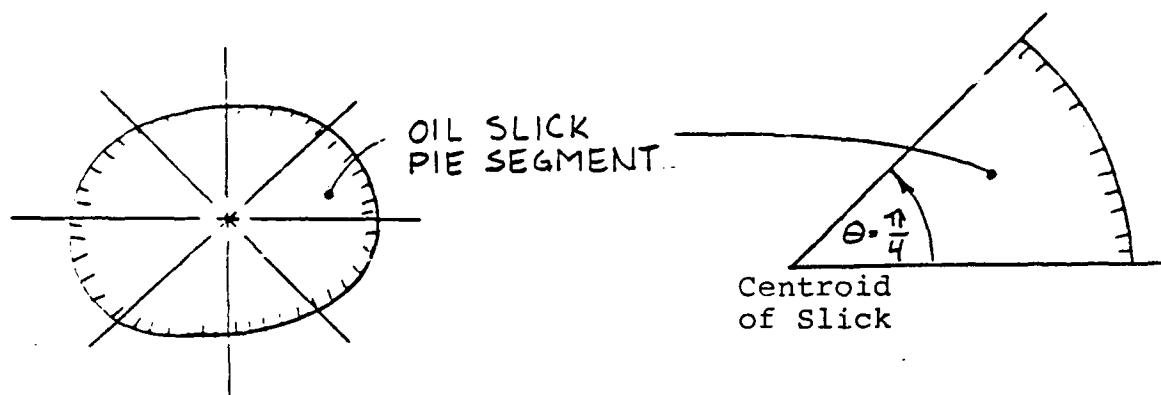
41

OIL SLICK
PIE SEGMENT

Centroid
of Slick

$\theta = \frac{\pi}{4}$

Fig. 12   Division of slick into pie segments

STRIP
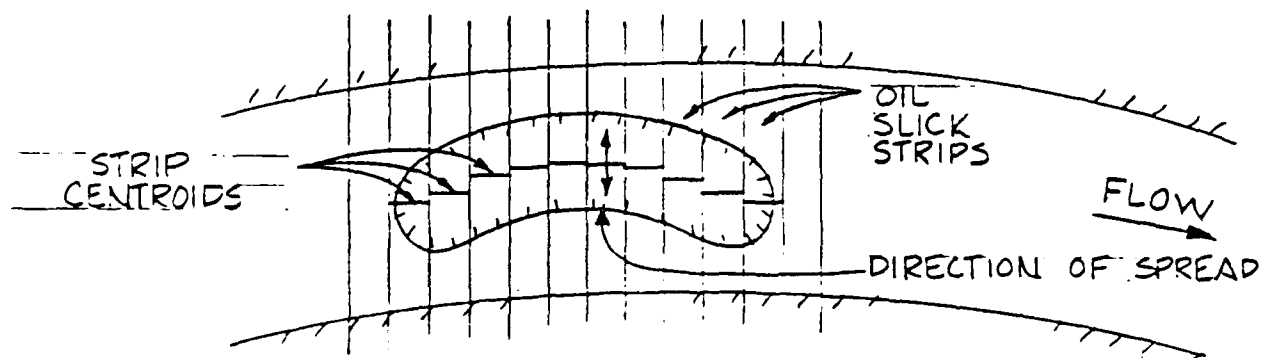CENTROIDS

OIL
SLICK
STRIPS

FLOW

DIRECTION OF SPREAD

Fig. 13   Division of slick into strips

42

slick, the rate of outward movement of an oil parcel along the radial direction, in a particular pie-shaped sector located at a distance r from the centroid of the slick can be calculated from the spreading rate of the mean radius $\bar{r}$ of the sector as $\frac{r}{\bar{r}} (\frac{d\bar{r}}{dt})$. Parcels scattered at distances far away from the main slick will be excluded from this process since small isolated patches of oil will not be subjected to the mechanical spreading. In this study, parcels which account for the outer 5% of the total slick volume are excluded in the mechanical spreading process. This is equivalent to excluding the parcels located at a radial distance greater than 2.2 $\bar{r}$ from the centroid of the slick. This was determined from numerical experiments for the spreading of circular slicks in a wide rectangular channel.

For an elongated slick, the rate of outward movement in the width direction of an oil parcel in a segment with mean length $\bar{\ell}$, located at a distance ℓ from the centroid of the segment, can be calculated from the rate of spreading of the mean length of the segment as $\frac{\ell}{\bar{\ell}} (\frac{d\bar{\ell}}{dt})$. Parcels accounting for the outer 5% of the slick volume are not subject to mechanical spreading.

Spreading Under Ice Cover

The spreading of oil under ice covers is a topic which has received little attention as compared to the open water case. However, the study of Hoult, et al. (1975) has provided some information. Results form their study suggest that appreciable mechanical spreading will only occur during continuous spills. For an instantaneous spill, the oil thickness is stabilized when the equilibrium thickness for the flow condition is reached.

43

There are no pressure gradients or surface tension forces to cause the further spreading of the oil. The oil reaches an equilibrium state in which cavities formed by the ice roughness contain a volume of oil which can decrease only with a significant increase in the current speed. Since a continuous spill will repeatedly add oil to fill the cavities, the excess oil will effectively spread to the empty neighboring cavities and establish an equilibrium state there. This is a crude but reasonable assessment since only the excess oil, from over-filling the cavities under the ice cover, would be expected to spread.

The formula used to model mechanical spreading for continuous spill under ice is:

$$r = 0.25 \ (\frac{\Delta g Q^2}{h'})^{1/6} \ t^{2/3} \tag{36}$$

where r = the slick radius; $\Delta = (\rho_w - \rho_o)/\rho_w$, the relative density ratio; g = the gravitational acceleration; Q = the average volume from the beginning of the spill. This equation is a result of balancing the frictional drag from the ice cover with the pressure drop that occurs as the oil flows into open cavities. In the simulaiton models, no mechanical spreading will occur for an instantaneous spill or once the continuous oil discharge stops. If the oil discharge is in progress, and the slick is nearly circular, the mechanical spreading will be calculated by Eq. 36.

44

II.6 Shoreline Boundary Conditions

An oil slick will reach a shoreline sometime after a spill occurs. Gundlach and Hayes (1978) proposed a method for classifying shorelines according to their "vulnerability"[1], which is the index reflecting the environmental sensitivity of the shoreline to the oil pollution. For beaches of different vulnerability Torgrimson (1974) suggested the use of "half-life" values to describe the ability of the shore to retain the oil. Half-life is a parameter which describes the 'absorbancy' of the shoreline, by describing the rate of re-entrainment of oil after it has landed at a given shoreline. Table 4 presents the half-life for different types of shorelines along with their vulnerability indices.

In the present model, the half-life concept is adopted. In this formulation, the volume of oil remaining on the beach can be related to its original volume by

$$V_2 = V_1 \, e^{-k(t - t)} \tag{37}$$

in which V_1 and V_2 = volumes of oil on the beach at time t_1 and t_2 respectively, and k = a decay constant. Since over one half-life, the volume of the oil on the beach will be reduced by half. The decay constant k can be expressed in terms of the half-life λ as:

---

[1] For some shorelines in the United States, ESI maps indicating types of shoreline characteristics are available. Maps for the Detroit/St. Clair river system are expected in the near future (T. Kaiser, NOAA, Ann Arbor, MI). This information can be used with the current model.

Table 4.   Shoreline descriptor and default parameters
           (Torgrimson, 1974)

SHORELINE DESCRIPTOR	HALF LIFE (hrs)	VULNERABILITY INDEX
Exposed Headland	1	1
Wave-Cut Platform	1	2
Pocket Beach	24	3
Sand Beach	24	4
Sand and Gravel Beach	24	5
Sand and Cobble Beach	8760	6
Exposed Tide Flats	1	7
Sheltered Rock Shore	8760	8
Sheltered Tide Flat	8760	9
Sheltered Marsh	8760	10
Land	8760	0

$$k = (-\ln(1/2))/\lambda \tag{38}$$

The fraction of the oil re-entrained into the water body during each time step is:

$$\frac{\Psi_1 - \Psi_2}{\Psi_1} = 1 - e^{-k\Delta t} = 1 - 0.5^{\Delta t/\lambda} \tag{39}$$

II.7 Evaporation

Evaporation can account for the largest loss in oil volume during the early stage of the slick transformation. In this study, the formulation developed by Mackay, et al. (1980) is used to calculate the rate of evaporation of the oil. The volume fraction of oil evaporated is determined as

$$F = (1/C)[\ln P_O + \ln(C K_E t + 1/P_O)] \tag{40}$$

where $E = K_E t$, is the "evaporative exposure" term, which varies with time and environmoental conditions; $K_E = K_M A v/(RTV_O)$, K_M = mass transfer coefficient, in m/s, $0.0025\ U_{wind}^{0.78}$; A = spill area, m^2; v = molar volume, m^3/mole; R = gas constant, 82×10^{-6} atm $m^3/(mol-^O K)$; T = surface temperature of the oil, $^O K$, which is generally close to the ambient air temperature, T_E in $^O K$; V_O = initial spill volume, m^3. The initial vapor pressure P_O in atm at the temperature T_E is

$$\ln P_O = 10.6 (1 - T_O/T_E) \tag{41}$$

in which, T_O = the initial boiling point, ^OK. The constant C can be determined by the relationship $T_E C$ = constant. C values for T_E = 283^OK and the initial boiling point, T_O, are given in Table 5. For crude oils of different API index values, C at T_E = 283^OK are given in Table 6 along with T_O. This table can be replaced by the following functional relationships obtained through curve fitting as shown in Figures 14 and 15.

$$C = 1158.9\ API^{-1.1435} \tag{42}$$

and

$$T_O = 542.6 - 30.275\ API + 1.565\ API^2 - 3439E\text{-}02\ API^3$$
$$+ 2.604E\text{-}04\ API^4 \tag{43}$$

The API index and the specific gravity of the oil are related by

$$\text{specific gravity} = 141.5/(API + 131.5) \tag{44}$$

The molar volume of oil is required in Eq. 40. The value of the molar volume can vary between 150×10^{-6} and 600×10^{-6} m^3/mole, depending on the composition of the oil. For fuel oils this value is approximately equal to 200×10^{-6} m^3/mole. The molar volume can be computed from the molecular weight of the oil. Typical values of molecular weights of various oil

Table 5. Suggested Evaporation Parameters for Various Petroleum
Fractions (T_E = 283°K) (Mackay, et al., 1980)

	T_O (°K)	C	P_O (atm)
Motor Gasoline			
Summer	314	5.99	.313
Winter	308	6.23	.39
Aviation Gasoline	341	2.81	.12
Diesel Fuel	496	5.57	3.4×10^{-4}
Jet Fuel	418	5.06	6.0×10^{-3}
No. 2 Furnace Oil	465	7.88	1.1×10^{-3}
Lube (heavy and light)	583	8.61	1.32×10^{-3}
Heavy Gas Oil	633	8.99	2.0×10^{-6}
Residuals	783	3.37	7.35×10^{-9}
Light Gas Oil	473	6.37	8.1×10^{-4}

TABLE 6. Suggested Evaporation Parameters for Various Crude Oils (T_E = 283°K)(Mackay, et al., 1980)

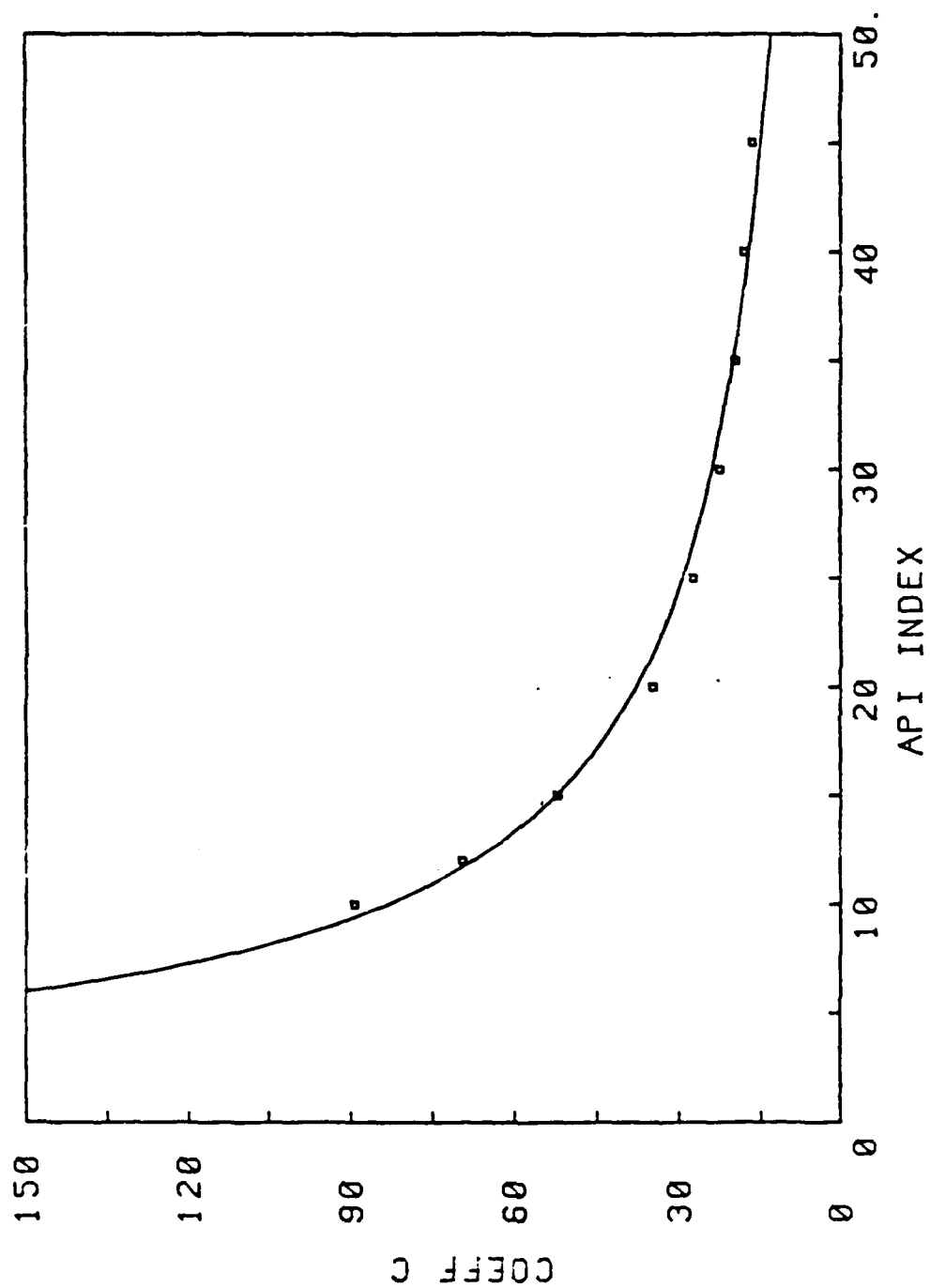| Gravity				
API	g/cm^3	C	T_O	P_O
10	1.0	89.2	366	0.044
12	.986	69.4	348	0.088
15	.966	52.1	339	0.13
20	.934	34.7	329	0.18
25	.904	27.2	330	0.17
30	.876	22.33	325	0.21
35	.850	19.5	314	0.31
40	.825	17.9	304	0.45
45	.802	16.4	283	1.004

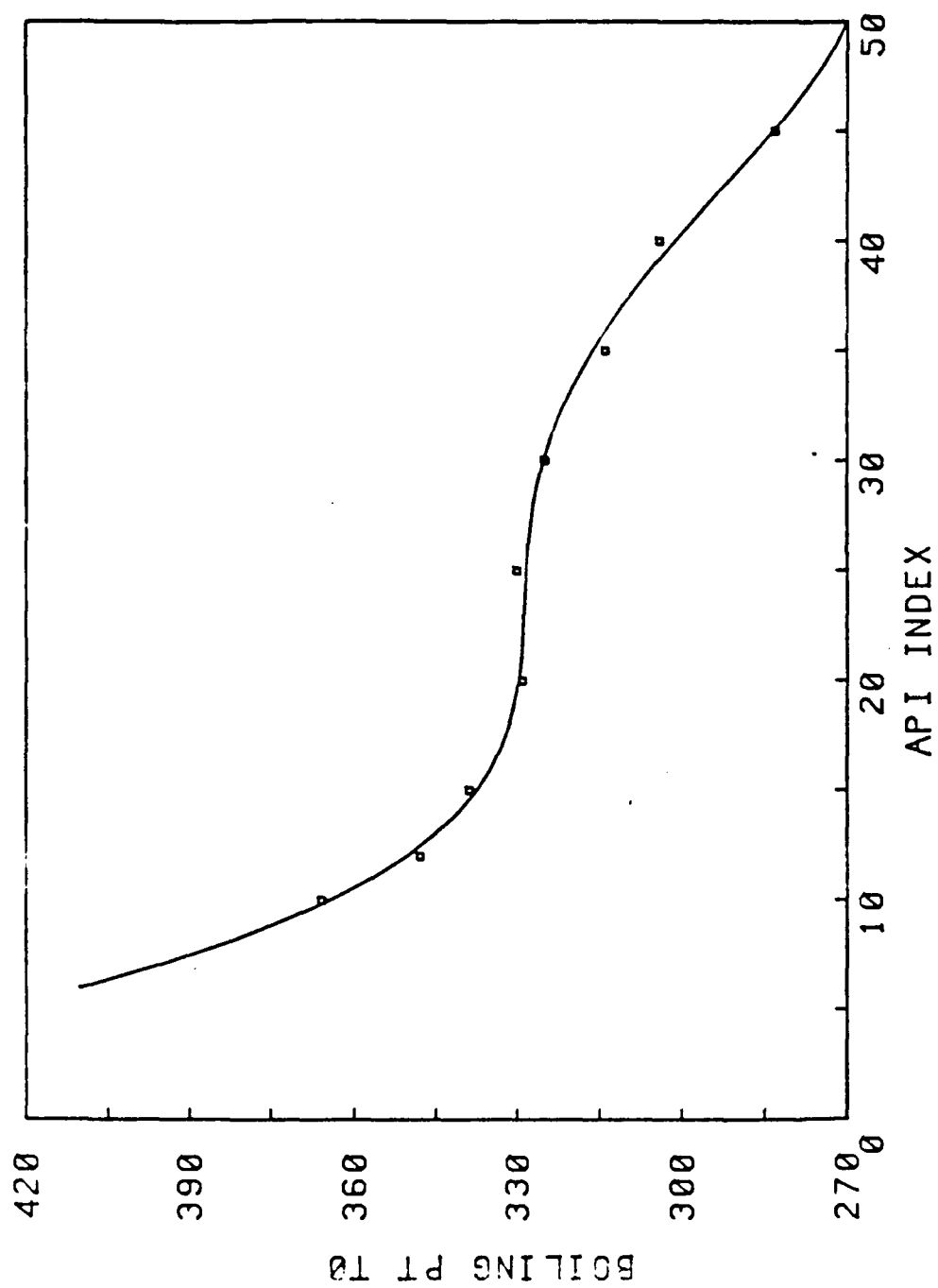Figure 14. Comparison of Eq. 42 with C values in Table 6

51

Figure 15. Comparison of Eq. 43 with T_o values given in Table 6.

52

components are given in Table 7. In Table 8, compositions of several different oils are given along with the concentration and molecular weight M_i of each component. Based on these the molecular volume can be computed from:

$$v = 1/\Sigma(c_i M_i) \qquad (45)$$

in which c_i = weight of the ith component per unit volume of oil.

II.8 **Dissolution**

Dissolution is an important process from the point of view of possible biological harm, although it accounts for a negligible fraction of the mass balance of the oil. Hydrocarbons which are likely to dissolve in the water are likely to evaporate. Dissolution, which tends to occur in the first few hours of a spill, thus has to compete with evaporation. Although solubility values for various hydrocarbon components are available, these values are difficult to utilize correctly for modeling purposes since they are often inconsistent for the same compounds.

In the present study, the method of Cohen, et al. (1980) is used. In this method the total dissolution rate N is calcualted by

$$N = K A_s S \qquad (46)$$

in which N = total dissolution rate of the slick, g/hr; K = a

53

TABLE 7. Basic Data for Oil Weathering
(Moore, et al., 1983)

Fraction	Description	% by wt. in Crude Oil	Density (gm/ml)	Boiling Point (C°)	Molecular Weight	Vapor Press. @ 20° C (mm)	Solubility (gm/10^5 gm Distilled H_2O)
1	Paraffin C_6-C_{12}	.1-20	.66-.77	69-230	86-170	110-.1	9.5-.01
2	Paraffin C_{13}-C_{25}	0^+-10	.77-.78	230-405	184-352	.1	.01-.004
3	Cycloparraffin C_6-C_{12}	5-30	.75-.9	70-230	84-164	100-1.	55-1.
4	Cycloparaffin C_{13}-C_{23}	5-30	.9-1.	230-405	156-318	1.-0	1.-0
5	Aromatic (Mono- and di-Cyclic) C_6-C_{11}	0-5	.88-1.1	80-240	78-143	72-.1	1780-0.
6	Aromatic (Poly-Cyclic) C_{12}-C_{18}	0^+-5	1.1-1.2	240-400	128-234	.1-0	12.5-0
7	Naphtheno-Aromatic C_9-C_{25}	5-30	.97-1.2	180-400	116-300	1.-0	1.-0
8	Residual (including heterocycles)	10-70	1.-1.1	> 400	300-900	0	0

54

Table 8. Estimated % Composition (by Weight) and
Comparison of Solubilities for Various
Petroleum Substances (Moore, et al., 1973)

Fraction	Description	Crude A	Crude B	#2 Fuel Oil	Kerosene	Bunker C
1	Alkanes (C_6-C_{12})	1	10	15	15	0
2	Alkanes $(C_{13}-C_{25})$	1	7	20	20	1
3	Cyclo-Paraffins(C_6-C_{12})	5	15	15	20	0
4	Cyclo-Paraffins$(C_{13}-C_{25})$	5	20	15	20	1
5	Mono- and Di-Cyclic Aromatics (C_6-C_{11})	2	5	15	15	0
6	Polycyclic Aromatics$(C_{12}-C_{18})$	6	3	5	2	1
7	Naphtheno-Aromatics(C_9-C_{25})	15	15	15	8	1
8	Residual	65	25	--	--	96
Estimated Maximum % Soluble		10	30	60	65	1
Estimated Maximum % Soluble Aromatic Derivatives		.1-10	.1-10	1-30	1-30	0-1
Reported % Soluble Aromatics Obtained in Seawater Extracts		.1	.01	,.1	.01	

dissolution mass transfer coefficient, assumed to be 0.01 m/hr; A_s = slick area, m^2; and S = the oil solubility in water. Huang and Montastero (1982) suggested that for a typical oil the solubility can be calculated by

$$S = S_o e^{-0.1t} \tag{47}$$

in which, S_o = the solubility for fresh oil and t = time in hours. Huang and Monastero (1982) suggested a typical value of 30 g/m^3 for S_o. The study of Lu and Polak (1973) provided more information on solubility. Lu and Polak formulated the rate of dissolution as

$$r_d = cde^{-dt} \tag{48}$$

in which r_d = rate of dissolution, mg m^{-2} day^{-1}. For three oil samples tested the coefficients c and d are given as shown in Table 9.

Table 9. Dissolution Coefficients at 25°C
(Lu and Polak, 1973)

Oil Type	API	c, mg m^{-2}	d, day^{-1}	$KS_o = cd$, gm^{-2}hr^{-1}
No. 2 fuel oil	35.5	1043	0.423	0.0184
Crude oil	38.6	8915	2.380	0.884
Bunker C oil	14.8	459	0.503	0.0104

CHAPTER III

RESULTS AND CONCLUSIONS

III.1 Model Applications

Based on the analytical formulation presented in Chapter II, two computer models are developed and applied to the connecting channels of the upper Great Lakes. These two models are named as ROSS (River Oil Spill Simulation) and LROSS (Lake and River Oil Spill Simulation), respectively. The program ROSS is developed for simulating oil spill in rivers and is applied to Detroit River, St. Clair River, lower St. Mary's River and upper St. Mary's River, as shown in Figs. 16, 17, 18 and 19. The model LROSS is developed for simulating oil spill in lake-river systems, and is applied to the Lake St. Clair-Detroit River system, as shown in Fig. 20. The details of the model structure, the flow chart, instructions for input data preparation, sample output, and program listing for both models are given in their user's manuals, which are Volumes II, III and IV of this report.

To illustrate the applicability of the computer models, three sample simulations are carried out and presented here. In all three cases fuel oil No. 2, with a specific gravity of 0.84 and a surface tension of 30 dynes/cm, has been selected as the spill material. The other input parameters for each case are summarized in Table 10. The results for these cases are shown graphically in Figs. 21 to 23. Evaporation characteristics used are $T_o = 465^\circ k$, $C = 7.88$, and $v = 2 \times 10^{-4}$ m^3/mole. Solubility

Table 10. Model Input Parameters for Sample Simulations.

River/Lake	Lower St. Mary's River	St. Clair River	Lake St. Clair -Detroit River
Model used	ROSS	ROSS	LROSS
No. of particles in the system	1000	1000	500
Spill Volums (gals)	8000	5000	10000
Spill Type	Continuous leak, duration = 30 min.	Instantaneous spill	Instantaneous spill
Flow Condition	High Flow (Q=111,000 cfs)	Low Flow (Q=130,000 cfs)	Median Flow (Q=184,000 cfs)
Wind Condition	0-4 hrs 5 mph from W 4-7 hrs 8 mph from E after 7 hrs, 10 mph from N	2 mph from W	2 mph from N
Air Temperature(°F)	50°F	70°F	50°F
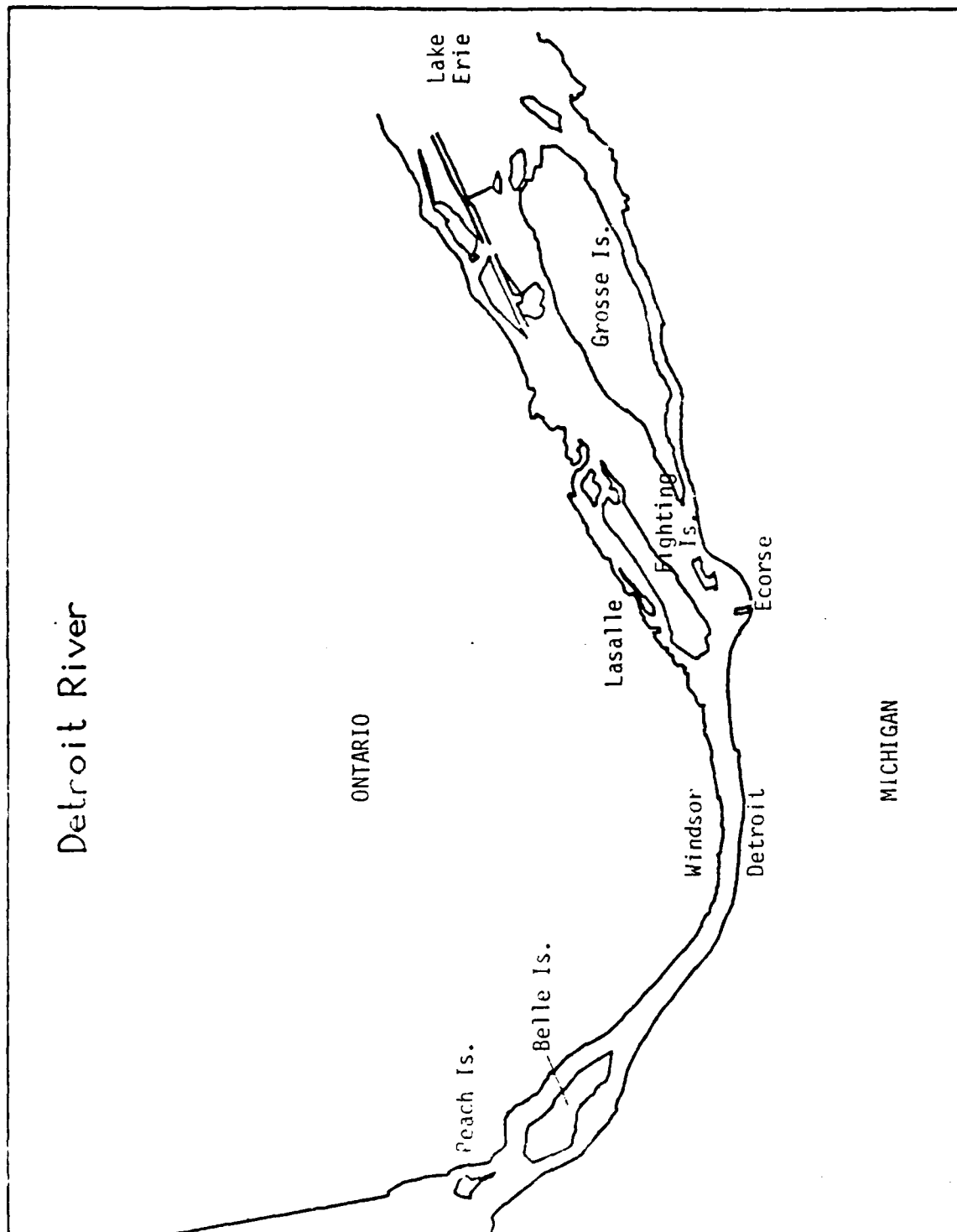
Figure 16. Detroit River.

60
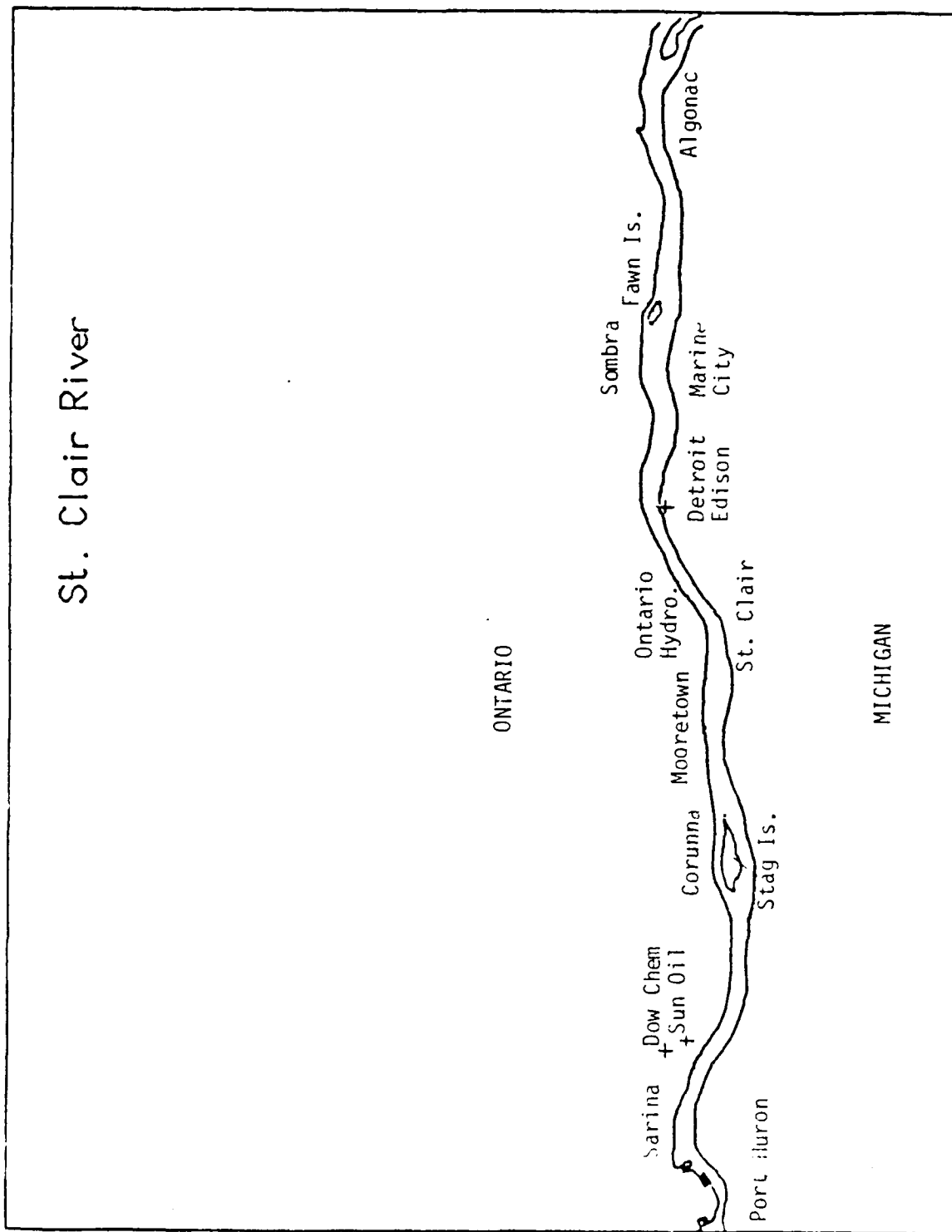
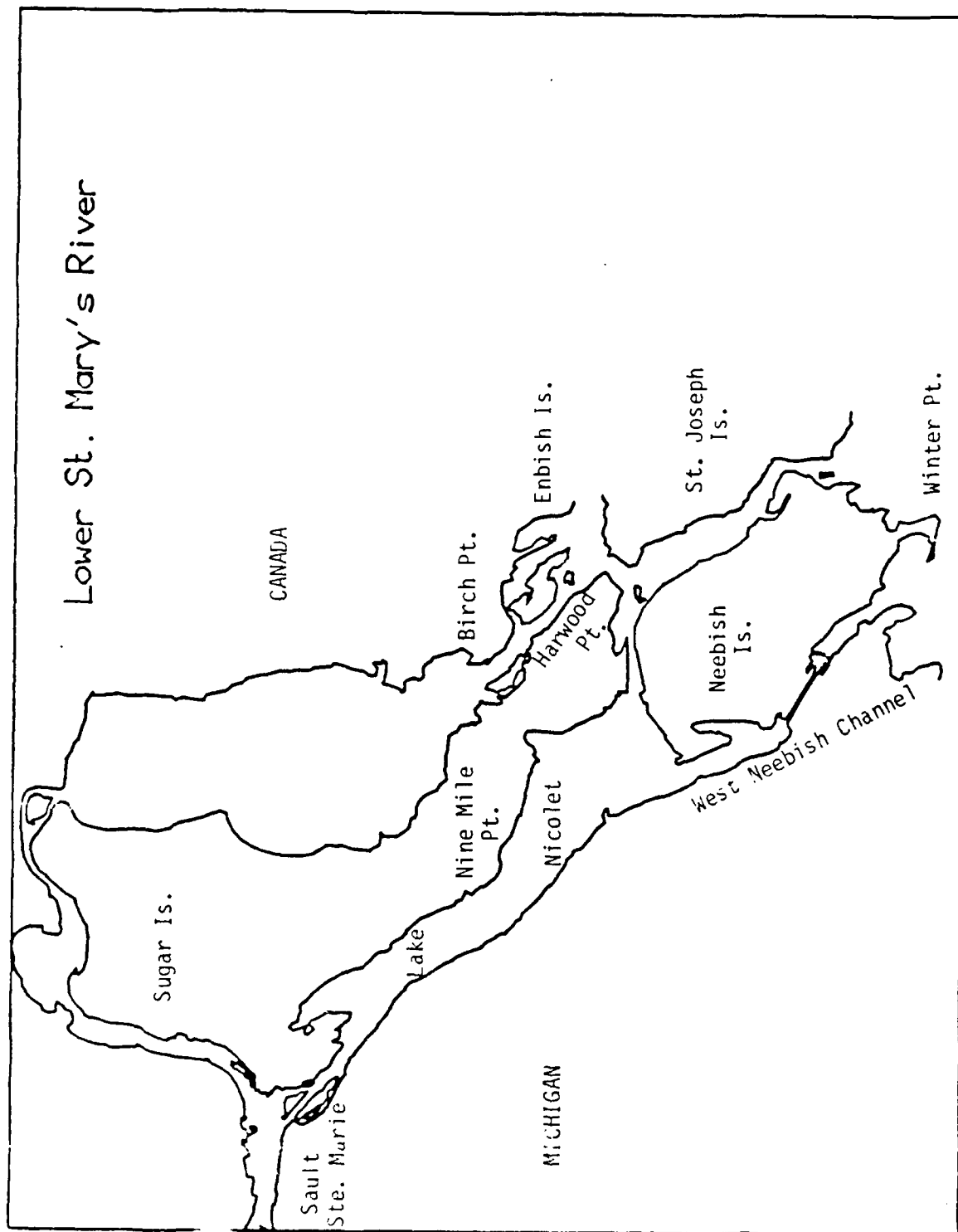# St. Clair River

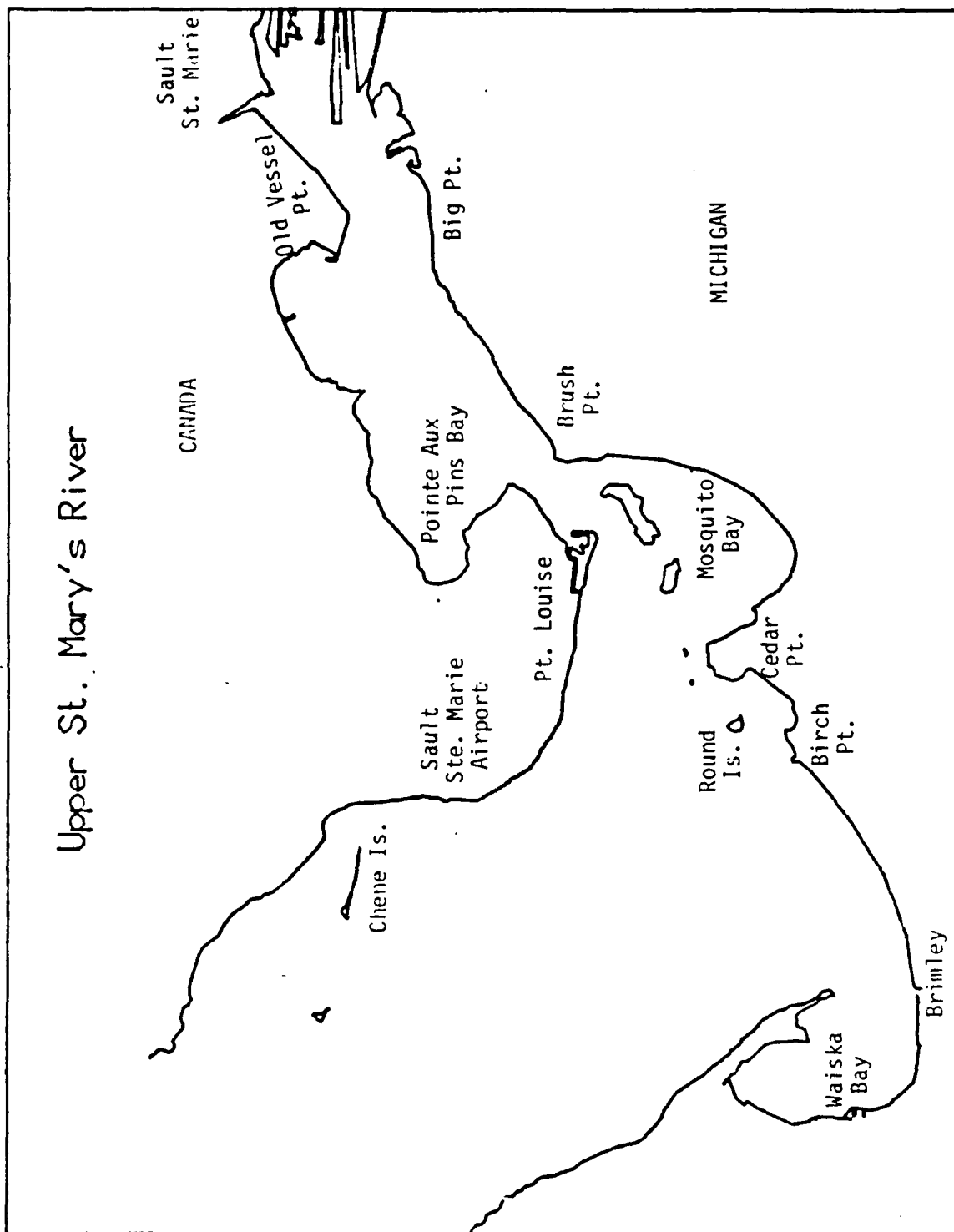Figure 17. St. Clair River.

Figure 18. Lower St. Mary's River.

62

Figure 19. Upper St. Mary's River.
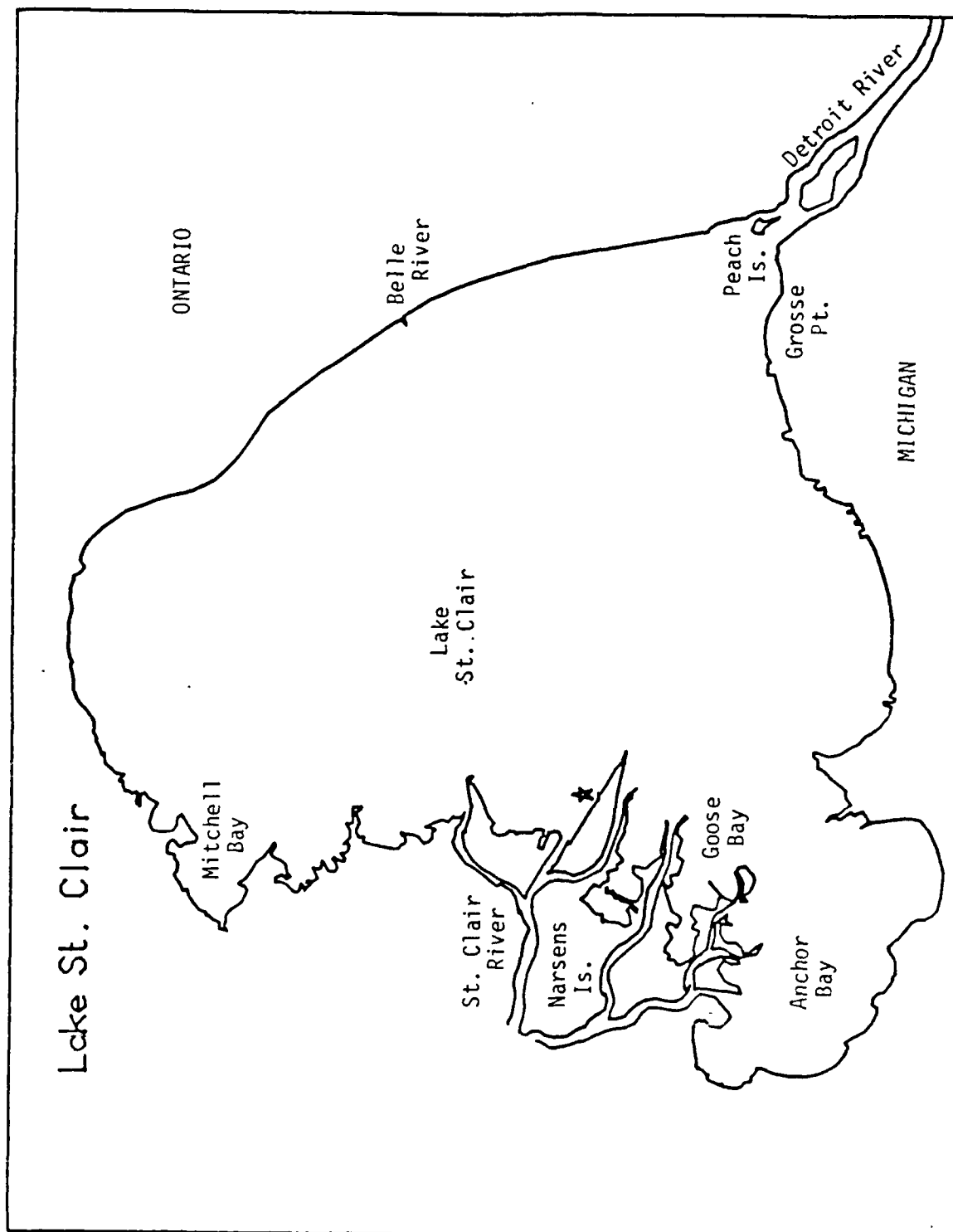
Figure 20. The Lake St. Clair-Detroit River System.

of the oil is assumed to be 0.1873×10^2 lb/ft^3. A time step of 15 minutes was used in all three simulations.

III.2 Summary and Conclusions

In this study, two-dimensional computer models for simulating oil slick movement in rivers and lakes are developed. The models are then applied to the connecting channels of the upper Great Lakes. In these models the oil slick is considered as a collection of discrete oil patches. The transformation of an oil slick due to advection, spreading, evaporation, and dissolution are considered. In open water regions the advection of oil patches in the slick are determined by the water current and wind using the drifting factor formulation. In ice covered regions, the advection of the oil is determined based on the empirical formula developed by Cox and Schultz (1981). The current distribution in the lake is determined by a rigid-lid circulation model (Schwab, et al. 1981). The current distribution in the river is determined by a stream-tube method. In the spreading process, mechanical spreading formulas developed by Fay (1969), Hoult (1972) are used. These formulas considered the balance of inertia, gravity, viscous and surface tension forces. In ice covered region the formula developed by Hoult, et al. (1975) is used. In addition to the mechanical spreading, the horizontal turbulent diffusion of the oil patches is simulated by a random walk formulation. Formulations developed by Mackay, et al. (1980) and Cohen, et al. (1980) are used to determine the rate
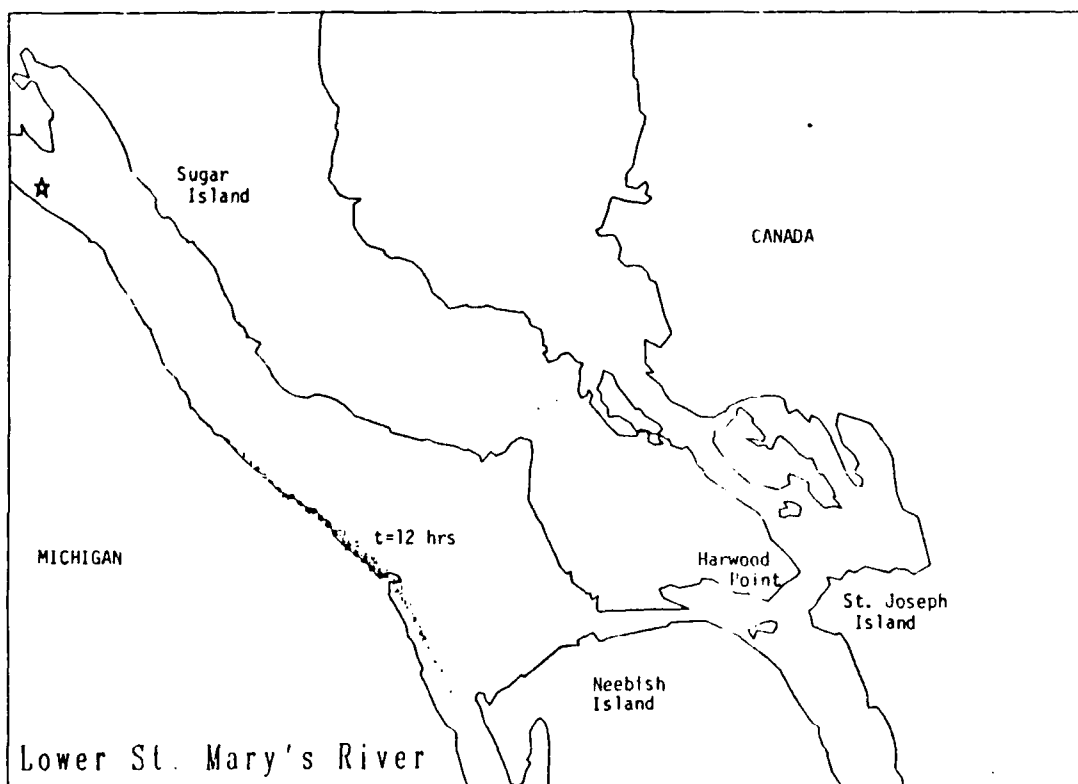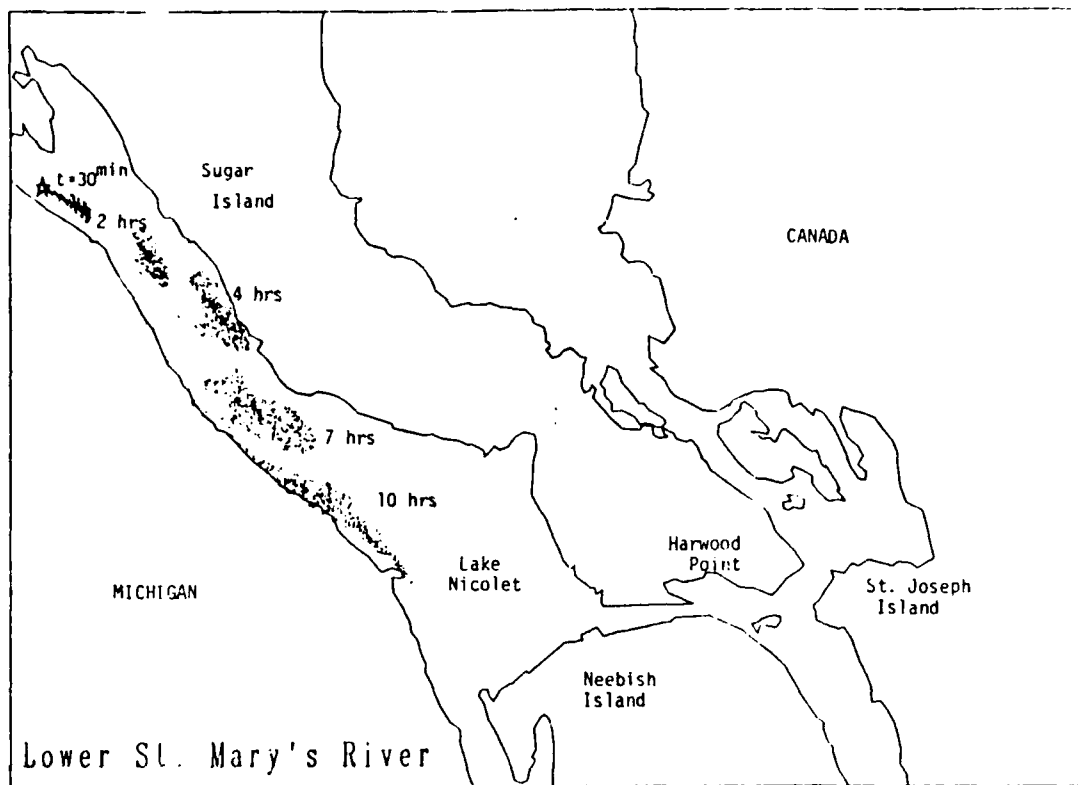
Figure 21.   Result of sample simulation — oil slick
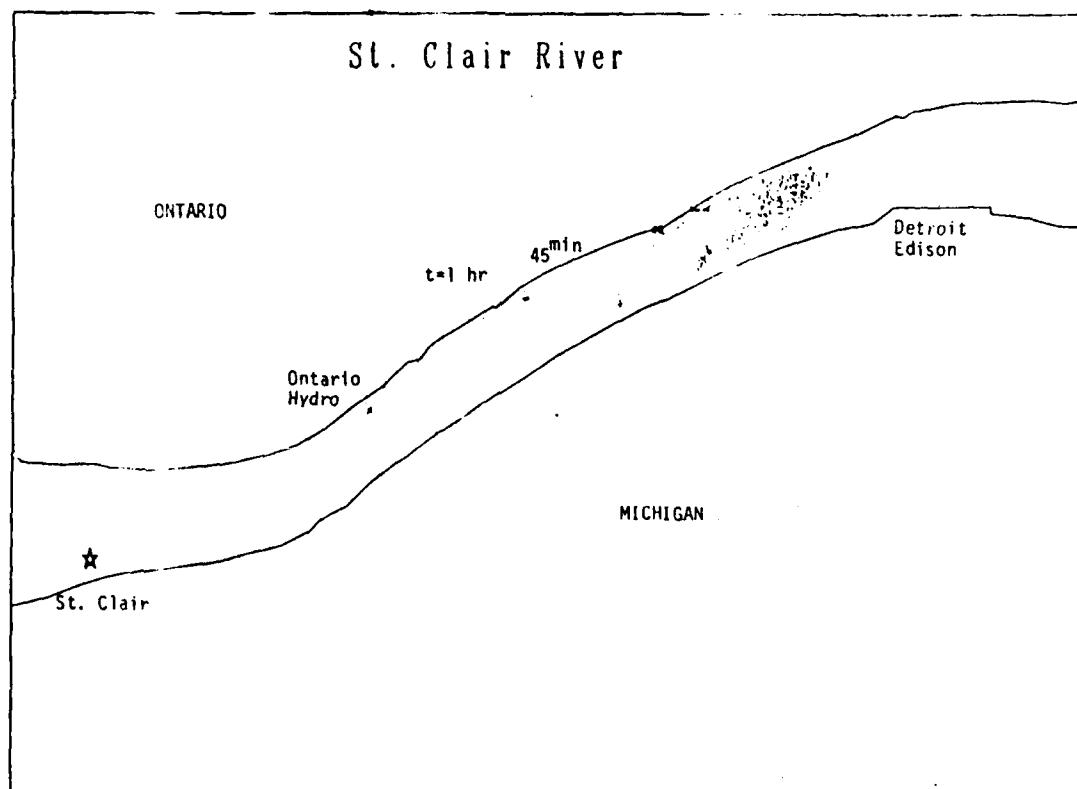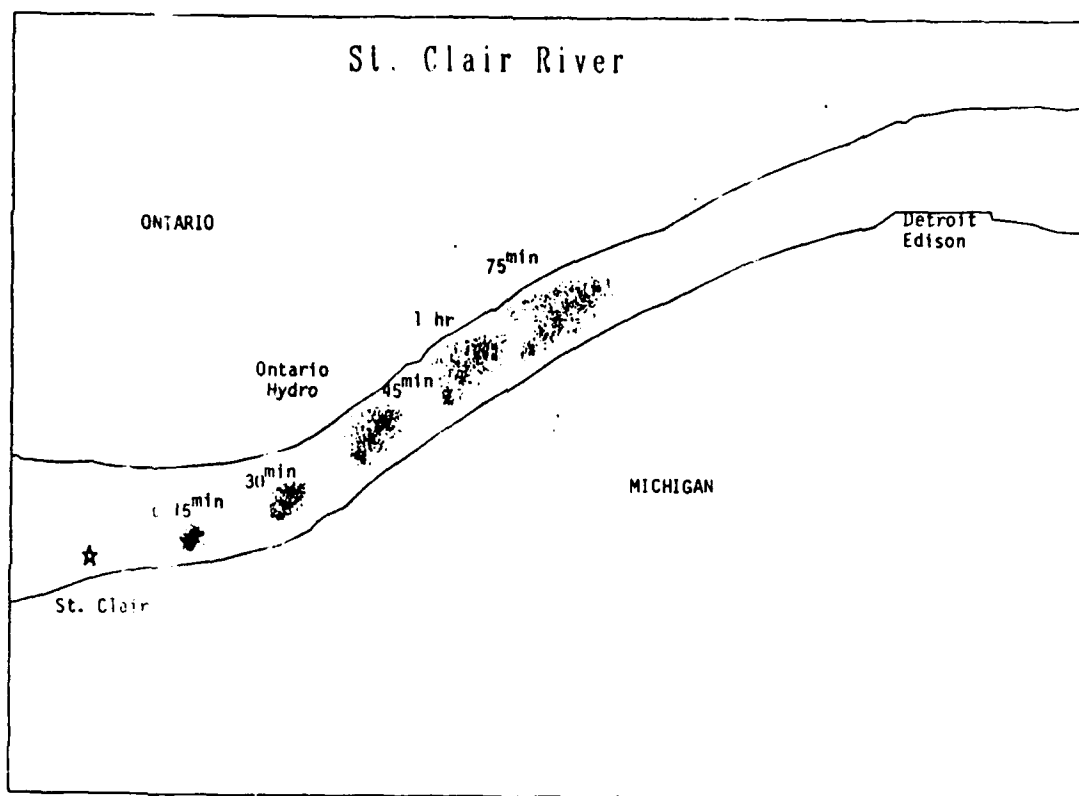transformation in lower St. Mary's River.

Figure 22.   Result of sample simulation-oil slick
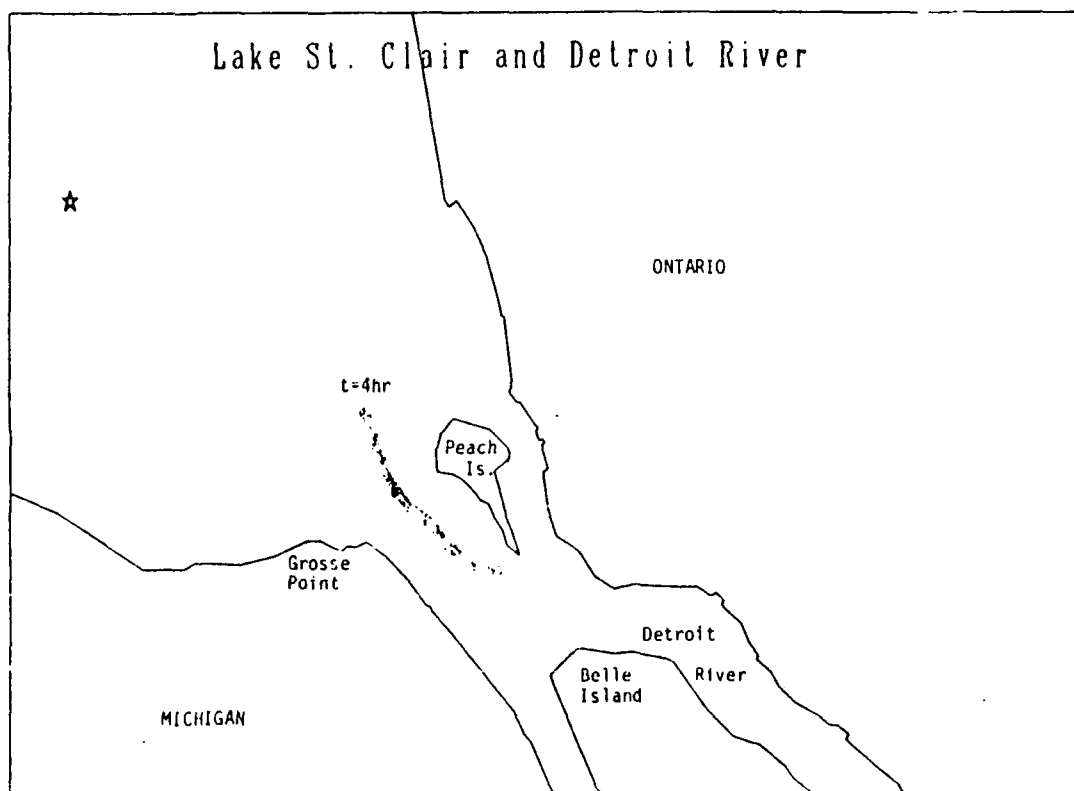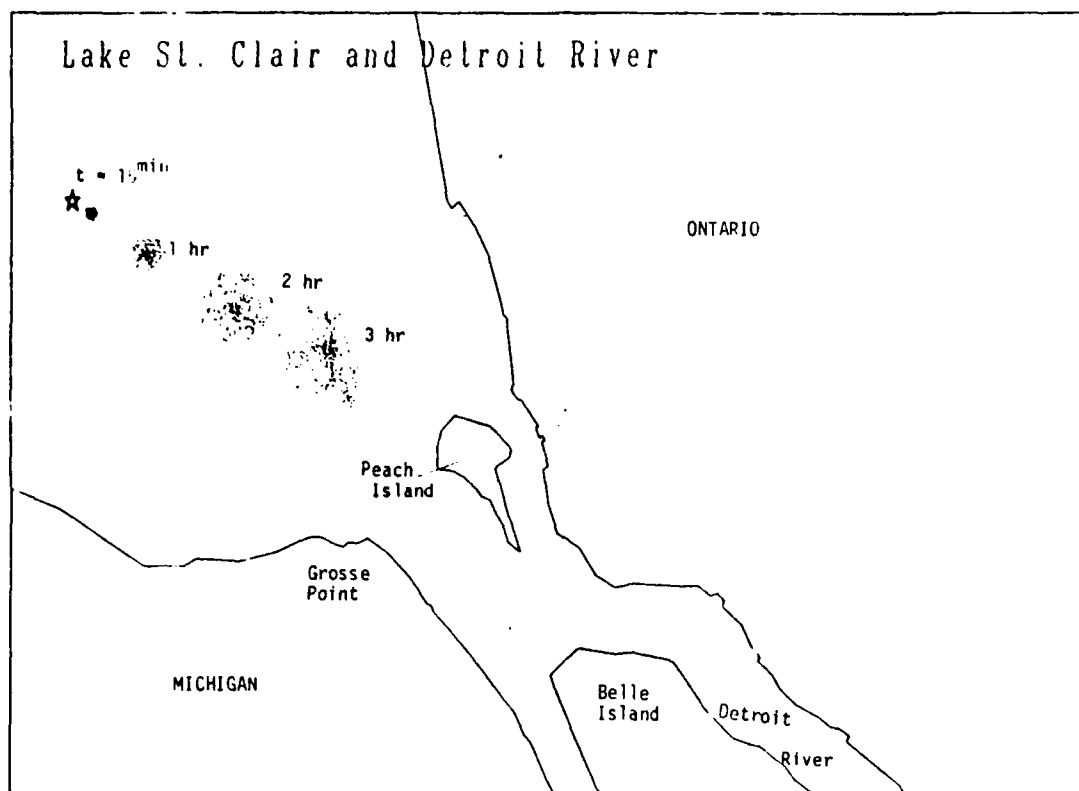   transformation in St. Clair River.

Figure 23.   Result of sample simulation-oil slick
transformation in the Lake St. Clair-
Detroit River system.

68

of evaporation and dissolution. Boundary conditions along the shore are formulated according to the oil retention capability of the shoreline.

The oil slick transformation model developed in this study contains as many processes as can be effectively and analytically modeled. In addition to computational efficiency, the model has several special features, including the ability of modeling instantaneous and continuous spills, the ability of realistically describe the irregular shapes of an oil slick, and the ability of accounting for the time-dependent variation of the flow conditions. Improvements on parts of the model are possible as better formulations on the oil slick transformation processes becomes available. The computer programs are designed so that refinement of the model elements and the expansion of the model to include additional slick transformation processes can easily be made.

REFERENCES

Ahlstrom, S.W., (1975). "A Mathematical Model for Predicting the Transport of Oil in Marine Waters," Battelle Pacific Northwest Laboratories, Richland, Washington.

Argiroff, C. and Weigum, L.E., (1986). "Great Lakes-Limited Season Extension," Proceedings, IAHR Ice Symposium, Iowa City, pp. 75-86.

Bennet, J.R., Clites, A.H., and Schwab, D.J., (1983). "A Two-Dimensional Lake Circulation Modeling System: Programs to Compute Particle Trajectories and the Motion of Dissolved Substances," NOAA Technical Memorandum ERL GLERL-46, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan.

Beurket, R.T., and Argiroff, C., (1984). "Great Lakes Limited Season Extension Operation of Sault Ste. Marie Locks, Michigan, U.S.A." IAHR Ice Symposium, Hamburg, Germany, pp. 267-276.

Bishop, P.L., (1983). Marine Pollution and Its Control, McGraw-Hill Book Co., 357 p.

Blokker, P.C., (1964). "Spreading and Evaporation of Petroleum Products on Water," Proceeding, 4th International Harbour Congress, Antwerp, pp. 911-919.

Boyd, J.D., (1979). "A Surface Spill Model for the Greak Lakes," Contribution No. 183, Great Lakes Environmental Research Laboratory, National Oceanic and Atmospheric Administration.

Butler, J., Morris, and Slecter, T., (1976). "The Fate of Petroleum in the Open Ocean," Sources, Effects and Sinks of Hydrocarbons in the Aquatic Environment, The American Inst. of Biological Sciences, pp. 287-297.

Cheng, R.T., Casulli, V., and Milford, S.N., (1984). "Eulerian-Lagrangian Solution of the Convection-Dispersion Equation in Natural Coordinates," Water Resources Research, 20(7), 944-952.

Cohen, Y., MacKay, D., and Shiu, W.Y., (1980)."Mass Transfer Rates Between Oil Slicks and Water," The Canadian Journal of Chemical Engineering, Vol. 58.

Cole, C.R., Foote, H.P., and Eliason, J.R., (1973). "Oil Spill Drift Forecasting Model," Technical Report, Battelle Pacific Northwest Laboratories, Richland, WA., 26 p. (Also paper presented at the Fourth Joint Chemical Engineering Conference, A.I.Ch.E., Vancouver, 1973).

Cox, J.C., and Schultz, L.A., (1981). "The Containment of Oil Spilled Under Rough Ice," Proceedings of the 1981 Oil Spill Conference, American Petroleum Institute, Washington, D.C., pp. 203-208.

DiPietro, N.D. and R.G. Cox, (1979). "The dynamics of spreading of oil on the surface of water," In, Workshop on the Physical Behavior of Oil in the Marine Environment (held at Princeton University).

Fannelop, T.K. and Waldman, G.D., (1972). "Dynamics of Oil Slicks," AIAA Journal, V. 10, pp. 506-510.

Fay, J.A., (1969). "The Spread of Oil Slicks on a Calm Sea," Oil on the Sea, (ed. by D. Hoult), pp. 53-64, Plenum, New York.

Fay, J.A., (1971). "Physical Processes in the Spread of Oil on a Water Surface," Proceedings of the Joint Conference on Prevention and Control of Oil Spills, Sponsored by API, EPA, and USCG, Washington, D.C., Amer. Petrol. Inst., pp. 463-467.

Fischer, H.B., et. al. (1979). Mixing in Inland and Coastal Waters, Academic Press, New York, p. 483.

Fingas, M., and Sydor, M., (1980). "Development of an Oil Spill Model for the St. Lawrence River," Technical Bulletin No. 116, Inland Waters Directorate, Water Management and Planning Branch.

Foda, M. and R.G. Cox, (1980). "The spreading of thin liquid films on a water-air interface," Journal of Fluid Mechanics (U.K.), V. 101, Part I, pp. 33-51.

Grubert, J.P., (1976). "Numerical Computation of Two-Dimensional Flows," Journal of the Waterways, Harbors and Coastal Engineering Division, ASCE, 102(WW1), 1-12.

Galt, J.A. and G.M. Torgrimson, (1979). "On-scene trajector modeling for the U.S. response to the Ixtoc-I blowout," Proceedings of the Workshop on Government Oil Spill Modeling, Princeton University and National Oceanic and Atmospheric Administration.

Gundlack, E.R., and Hayes, M.D., (1978). "Vulnerability of Coastal Environments to Oil Spill Impacts," Marine Tech. Society Journal, Vol. 12, No. 4, pp. 18-27.

Hamilton, G.D., Soileau, C.W., and Stroud, A.D., (1982). "Numerical Modeling Study of Lake Pontchautrain," Journal of the Waterways, Ports, Coastal and Ocean Division, ASCE, 108(WWI), 49-64.

Hoult, D.P., (1972). "Oil Spreading on the Sea," Annual Review of Fluid Mechanics, V.   , p. 341-367.

71

Hoult, D.P. and Suchon, W., (1970). "The Spread of Oil in a Channel," Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Hoult, D.P., Wolfe, S., O'Dea, S., and Patureau, J.P., (1975). "Oil in the Arctic," Report No. CG-D-96-75, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Huang, J.C., (1983). "A Review of the State-of-the-Art of Oil Spill Fate/Behavior Models," Proceedings of the 1983 Oil Spill Conference, American Petroleum Institute, Washington, D.C., pp. 313-322.

Huang, J.C. and Monastero, F.C., (1982). "Review of the State-of-the-Art of Oil Spill Simulation Models," Final Report submitted to the American Petroleum Institute.

Hunter, J.R., (1980). "An interactive computer model of oil slick motion," Proceedings, Oceanology International '80 (U.K.), pp. 42-50.

Jordon, R.E. and Payne, J.R., (1980). Fate and Weathering of Petroleum Spills in the Marine Environment, Ann Arbor Science, Ann Arbor, Michigan, 174 p.

Kerr, C. and K. Babu, (1970). "The collapse of a column of fluid onto a horizontal surface," In, Workshop on the Physical Behavior of Oil in the Marine Environment, Princeton University.

Leendretse, J.J., (1970). "A Water-Quality Simulation Model for Well-Mixed Estuaries and Coastal Seas: Vol. I, Principles of Computation," Report RM-6230-RC, The Rand Corporation, Santa Monica, California, 71 p.

Lou, C.Y., and Polak, J., (1973). "A Study of Solubility of Oil in Water," Report EPS-4-EC-76-1, Environmental Protection Service, Canada, 25 p.

Mackay, D., Paterson, S., and Nadeau, S., (1980). "Calculation of the Evaporation Rate of Volatile Liquids," Proceedings, National Conference on Control of Hazardous Material Spills, Louisville, KY, pp. 361-368.

Mackay, D., Paterson, S., and Trudel, K., (1980). "A Mathematical Model of Oil Spill Behavior," Environmental Protection Service, Fisheries and Environment Canada.

Madsen, O.S., (1977). "A realistic model of the wind-induced Ekman boundary layer," Journal of Physical Oceanography, 7, N2, pp. 248-255.

Moore, S.F., Dwyer, R.L., and Katz, A.M., (1973). "A Preliminary Assessment of the Environmental Vulnerability of Machias Bay, Maine to Oil Supertankers," Report No. 162, R.M. Parsons Lab., MIT, pp. 59.

Murray, S.P., (1972). "Turbulent Diffusion of Oil in the Ocean," Liminology and Oceanography, Vol. 17, No. 5, pp. 651-660.

Okubo, A., (1962). "A Review of Theoretical Models of Turbulent Diffusion in the Sea," Technical Report 30, Chesapeake Bay Institute, The Johns Hopkins University, p. 105.

Petroski, M.E., (1985). "A Mathematical Model for an Oil Spill in Lakes and Rivers," M.S. Thesis, Department of Civil and Environmental Engineering, Clarkson University, Potsdam, NY, p. 329.

Petroski, M.E. and Glebas, T., (1985). "Microcomputer Digitizing of River Geometry for Hydraulic Modeling," Third National Conference on Microcomputers in Civil Engineering, Orlando, Florida.

Rasmussen, D., (1985). "Oil Spill Modelig - A Tool For Cleanup Operations," Proceedings of the 1985 Oil Spill Conference, American Petroleum Institute, Washington, D.C., pp. 243-249.

Roache, R.J., (1972). Computational Fluid Dynamics, Hermosa Publishers, Albuquerque, N.M.

Rouse, H., (1946). Elementary Fluid Mechanics, John Wiley & Sons, Inc., N.Y., pp. 360.

Sayre, W.W. and Chang, F.M., (1968). "A Laboratory Investigation of Open-Channel Dispersion Processes for Dissolved, Suspended, and Floating Dispersants," Professional Paper 433-E, U.S.G.S., p. 71.

Schwab, D.J. and Sellars, D.L., (1980). "Computerized Bathymetry and Shorelines of the Great Lakes," NOAA Data Report ERL GLERL-16, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan.

Schwab, D.J., Bennet, J.R., and Jessup, A.T., (1981). "A Two-Dimensional Lake Circulation Modeling System," NOAA Technical Memorandum ERL GLERL-38, Great Lakes Environmental Research Laboratory, Ann Arbor, Michigan.

Schwab, D.J., Bennet, J.R., and Lynn, E.W., (1984). "'PATHFINDER' -- A Trajectory Prediction System for the Great Lakes," NOAA Technical Memorandum ERL GLERL-53, Great Lakes Environmentalk Research Laboratory, Ann Arbor, Michigan.

Schwartzberg, H.G., (1971). "The Movement of Oil Spills," Proceeding, Joint Conference on Prevention and Control of Oil Spills, API, pp. 489-494.

Shen, H.T. and Ackermann, N.L., (1980). "Wintertime Flow Distribution in River Channels," _Journal of the Hydraulics Division_, ASCE, Vol. 106, No. HY5, pp. 805-817.

Stolzenbach, K.D., Madsen, O.S., Adams, E.E., Pollack, A.M. and Cooper, C.K., (1977). "A Review and Evaluation of Basic Techniques for Predicting the Behavior of Surface Oil Slicks," _Report No. 22_, Department of Civil Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts.

Thomas, R., (1984). "Unsteady Flow Model for Great Lakes Connecting Channels," unpublished, Department of the Army, Detroit District Corp of Engineers, Detroit, Michigan (Personnel Communication).

Tsahalis, D.T., (1979). "Theoretical and Experimental Study of Wind and Wave-Induced Drift," _Journal of Physical Oceanography_, V. 9, pp. 1243-1257.

Tsahalis, D.T., (1979). "Contingency planning for oil spills: RIVERSPILL-a river simulation model," _Proceedings of the 1979 Oil Spill Conference_, American Petroleum Institute, Washington, D.C.

Torgrimson, G.M., (1984). "The On-Scene-Spill Model: A User's Guide," NOAA Hazardous Materials Response Branch, Technical Report, unpublished manuscript.

U.S. Army Corps of Engineering, Detroit District, (1974). "Detroit River Aerial Drogue Survey and Mean Velocity Distribution Study," _River Current Studies_, Great Lakes Hydraulics and Hydrology Branch.

Waldman, G.A., Johnson, R.A., and Smith, P.C., (1973). "The Spreading and Transport of Oil Slicks on the Open Ocean in the Presence of Wind, Waves, and Currents," _Coast Guard Report No. CG-D-17-73, AD-763 926_, 70 pp.

Wheeler, R.B., (1978). _The Fate of Petroleum in the Marine Environment_, Special Report, Exxon Production Research Co.